

# Recommended Vapor–Liquid Equilibrium Data. Part 3. Binary Alkanol–Aromatic Hydrocarbon Systems

Marian Góral, Adam Skrzecz, Andrzej Bok, and Andrzej Mączyński<sup>a)</sup>

Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

Paweł Oracz

Department of Chemistry, University of Warsaw, Warsaw, Poland

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The recommended vapor–liquid equilibrium (VLE) data for mixtures of alkanols with benzene and alkylbenzenes have been selected after critical evaluation of all data reported in the open literature up to the middle of 2002. The evaluation procedure consisted in combining the thermodynamic consistency tests, data correlation, comparison with enthalpy of mixing data, and comparison of VLE data for various mixtures. The data were correlated with equations based on local compositions concept as well as with equation of state appended with chemical term (EoSC) proposed by Góral. The recommended data for 29 systems are presented in the form of individual pages containing tables of data, figures and auxiliary information. Each page corresponds to one system and contains three isotherms (spaced by at least 15 K) and one isobar (preferably at 101.32 kPa). Experimental gaps were completed with the predicted data. © 2004 American Institute of Physics. [DOI: 10.1063/1.1760761]

Key words: alkanols; aromatic hydrocarbons; binary systems; predicted data; recommended data; vapor–liquid equilibria.

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<sup>a)</sup>Author to whom correspondence should be addressed. Electronic mail: macz@ichf.edu.pl

## 1. Introduction

The objective of this paper is to provide selected and critically evaluated vapor–liquid equilibrium (VLE) data for binary mixtures of alkanols with benzene and alkylbenzenes. It is a continuation of our presentations on recommended binary VLE data in this journal. The *n*-alkanol-*n*-alkane systems were described in Part 1.<sup>1</sup> The remaining alkanol–alkane systems were presented in Part 2.<sup>2</sup> All available data (below 0.5 MPa) for considered systems were taken from the open literature up to the middle of 2002. They consist of 766 data sets taken from 229 references, listed in Appendix 1 (Sec. 8). The data were critically evaluated using multistage procedure. Details were described in Part 1 of this series.<sup>1</sup> The procedure consists of combining the thermodynamic consistency test, data correlation, comparison with enthalpy of mixing, and comparison of VLE data for various mixtures and series of mixtures.

## 2. Correlation of VLE Data

Correlations of the data were done with equation of state with a chemical term (EoS) method developed by Góral.<sup>3</sup> The same method was used in previous parts. EoS was used also for an accurate description of VLE in alcohol–hydrocarbon systems published elsewhere.<sup>4,5</sup>

EoS uses Redlich–Kwong equation of state<sup>6</sup> appended with the association term. The EoS, having one adjustable binary parameter, is capable of correlating the investigated systems as accurately as the two-parameter Wilson equation. The method of correlation was described before in Part 1.<sup>1</sup>

Whenever possible the saturated vapor pressures reported by the authors of data were used. If saturated vapor pressures were not reported or in the case of isobaric data, then saturated data vapor pressures were calculated from Antoine's equation whose parameters were taken from the Thermodynamic Research Center.<sup>7</sup>

The correlating equations depend on the model of association. Self-association of *i*th alkanol is characterized by the equilibrium constant  $K_{ii}$ . The temperature dependence of  $K_{ii}$  is approximated with the van't Hoff equation:

$$K_{ii} = K_{ii}^0 \exp[(-\Delta H_i/R)(1/T - 1/313.15)], \quad (1)$$

where  $K_{ii}^0$  is the equilibrium constant at 313.15 K and  $\Delta H_i/R$  is enthalpy of the association divided by the gas constant.

Excluded volumes of the alkanols ( $b_i$ ), used in the chemical part of EoS, are shifted by some value  $\Delta b_i$  in respect to excluded volume used in the Redlich–Kwong EoS.

Parameters of alkanols ( $K_{ii}^0$ ,  $\Delta H_i$ , and  $\Delta b_i$ ) are the same as those used before. They are given in Table 1. Only  $K_{ii}^0$  for ethanol was changed. Previously  $K_{ii}^0$  for ethanol was the same as those used for higher 1-alkanols. Now ethanol has an intermediate value of  $K_{ii}^0$  between methanol and higher 1-alkanols. The actual value of  $K_{ii}^0$  gives significantly better

TABLE 1. Parameters of the self-association model of alkanols: enthalpy of self-association divided by gas constant ( $\Delta H/R$ ), constant of self-association at 313.15 K ( $K_{ii}^0$ ), and  $\Delta b_i$  calculated from number of carbon atoms of the alkanol ( $N_i$ )

$-\Delta H/R$	$K_{ii}^0/\text{MPa}^{-1}$	$\Delta b_i/\text{cm}^3$	Alkanol
2700	0.850	2.1	Methanol
2700	0.650	-3.3	Ethanol
2700	0.470	9.0(2-N <sub>i</sub> )	1-Alkanols C <sub>i</sub> H <sub>2<i>i</i>+1</sub> OH ( <i>i</i> >2)
2700	0.335	9.0(2-N <sub>i</sub> )	2-Alkanols
2700	0.250	9.0(2-N <sub>i</sub> )	3-Alkanols

correlation of the ethanol mixtures recommended in this paper and assures good correlation of the mixtures investigated in the previous parts of this paper series.<sup>1,2</sup>

It was found that a weak cross association between the alkanols and the aromatic compounds must be taken into account. The model of the association and the relevant equations were described by Góral.<sup>1</sup> In the first stage of this investigation  $K_{ij}$  was treated as adjustable parameter in EoS. Analysis of  $K_{ij}$  fitted individually to each VLE data set showed that it can be approximated with Eq. (2)

$$K_{ij} = (\alpha K_{ii})^{0.5}, \quad (2)$$

where  $K_{ii}$  is expressed with Eq. (1). In further calculations  $\alpha=0.000\ 80\ \text{MPa}^{-1}$  was used.

## 3. Prediction of VLE Data

The main advantage of EoS is that it uses only one adjustable binary parameter ( $\Theta$ ) for correlation of VLE.  $\Theta$  is used in the mixing rule for energetic parameter in the equation of state. In Parts 1 and 2 of this publication series<sup>1,2</sup> semiempirical formulas for prediction of  $\Theta$  in the relevant mixtures were proposed.

In this work the prediction of VLE is based on excess Gibbs energy at equimolar concentration. This quantity ( $G_{0.5}^E$ ) divided by the gas constant ( $R$ ) and temperature ( $T$ ) is denoted here by  $Q$

$$Q \equiv G_{0.5}^E/RT. \quad (3)$$

$Q$  is related to  $\Theta$  via equations for chemical potentials yielded by EoS (see Part 1<sup>1</sup>). If a value of  $Q$  is known, then the value of  $\Theta$  for the corresponding mixture can be determined and after that VLE can be calculated with EoS. Thus the problem of VLE prediction is reduced to the prediction of  $Q$ . In order to develop rules for the prediction the values of  $Q$  determined from experimental VLE data sets were selected and analyzed.

The advantage of using  $Q$  is that it is not confined to the equation used for the correlation of the VLE data. Moreover temperature dependence of  $Q$  in a simple way depends on the heat of mixing. This dependence is described by the Gibbs–Helmholtz equation

$$\partial Q / \partial (1/T)|_p = H_{0.5}^E/R, \quad (4)$$

TABLE 2. Parameters for calculation of heat of mixing. Values of  $B/C$  used in Eqs. (5) and (6) adjusted to  $H^E$  data

	Benzene	Toluene	Ethylbenzene	<i>p</i> -Xylene
Methanol	75/1.4	76/1.6	83/1.7	80/1.6 <sup>a</sup>
Ethanol	93/1.7	87/2.0	94/2.0	90/1.9
1-Propanol	114/1.9	106/2.1	111/2.2	108/2.1 <sup>a</sup>
1-Butanol	125/1.8	113/1.9	115/2.2	110/1.9 <sup>a</sup>
1-Pentanol	121/1.7	110/1.8	112/1.9	103/1.8 <sup>a</sup>
1-Hexanol			106/1.8 <sup>c</sup>	97/1.7 <sup>a</sup>
2-Propanol	155/2.0	144/2.1	146/2.2	138/2.1 <sup>a</sup>
2-Butanol	172 <sup>b</sup> /2.0 <sup>a</sup>	161 <sup>b</sup> /2.1 <sup>a</sup>		
3-Pentanol	189 <sup>c</sup> /2.0 <sup>a</sup>			
2-Methyl-1-propanol	157/2.0	148 <sup>b</sup> /2.1 <sup>a</sup>	150 <sup>c</sup> /2.2 <sup>a</sup>	142 <sup>c</sup> /2.1 <sup>a</sup>
2-Methyl-2-propanol	166 <sup>b</sup> /2.0 <sup>a</sup>	154 <sup>b</sup> /2.1 <sup>a</sup>	156 <sup>c</sup> /2.2 <sup>a</sup>	
2-Methyl-2-butanol	188/2.0 <sup>a</sup>			

<sup>a</sup>Estimates.

<sup>b</sup>Adjusted to VLE data.

<sup>c</sup>Interpolated in series of mixtures.

where  $H_{0.5}^E$  is the equimolar heat of mixing. Equation (4) was integrated with the assumption that  $H_{0.5}^E$  is a linear function of temperature

$$H_{0.5}^E/R = B + C(T - 298.15). \quad (5)$$

The integration of Eq. (4) yields Eq. (6)

$$Q = A + B(1/T - 1/T_0) + C[298.15/T - 298.15/T_0 - \ln T_0/T], \quad (6)$$

where  $A$  is the value of  $Q$  at the reference temperature  $T_0 = 313.15$  K.

In order to compare various data sets reported for the same system they were correlated with EoS and from each data set the corresponding value of  $Q$  was determined. Next these  $Q$  values were plotted versus  $T$  and approximated with Eq. (6), where  $A$  was treated as an adjustable parameter. Whenever possible  $B$  and  $C$  adjusted to  $H^E$  data were used in Eq. (6). If  $H^E$  data for given system were not reported then  $B$  was also adjusted to the experimental  $(T, Q)$  points. In this case we adopted the value of  $C$  taken from similar mixtures. It was justified by the fact that  $C$  has almost the same value in the investigated systems (with the exception of methanol and ethanol mixtures). The bibliography of the  $H^E$  is given in Appendix 2 (Sec. 9). The obtained values of  $B$  and  $C$  are given in Table 2.

The plots of  $Q$  versus  $T$  were used for checking consistency between the experimental  $Q$  values and  $H^E$  data, which helped to identify the outlying VLE data sets. Using these plots and Eq. (6), values of  $A$  for 34 systems were selected. They were further analyzed in order to check consistency in series of mixtures. It was found that mixtures of the *n*-alkanols with the aromatic compounds fulfill a simple empirical formula:

$$A_{ij} = 0.2460 + 0.1507[(N_j + 1)^{0.5} - N_i^{0.5}], \quad (7)$$

where  $A_{ij}$  is value of  $Q$  for  $i$ th alkanol and  $j$ th aromatic hydrocarbon at 313.15 K,  $N_i$  and  $N_j$  are corresponding numbers of carbon atoms. For isomeric alkanols  $N_i$  was adjusted

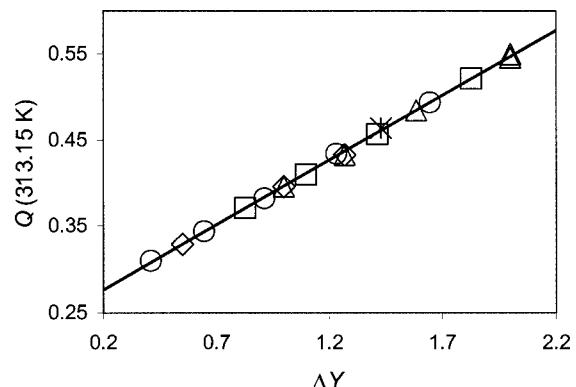


FIG. 1. Values of  $Q$  at 313.15 K for mixtures of *n*-alkanols with benzene (circles), toluene (squares), xylenes (triangles), ethylbenzene (diamonds), and mesitilene (stars) plotted vs  $\Delta Y = (N_j + 1)^{0.5} - N_i^{0.5}$  and the line calculated with Eq. (7).

to experimental values of  $A_{ij}$  via Eq. (7). In this case the same value of the adjusted  $N_i$  was used for all mixtures of a given alkanol with various aromatic hydrocarbons. The accuracy of Eq. (7) is illustrated by Figs. 1 and 2.

Equation (7) solves the problem of the VLE prediction at 313.15 K. For a prediction at other temperatures the corresponding  $Q$  values were obtained by extrapolation. The extrapolation was done by means of Eq. (6) using  $A$  determined with Eq. (7) and parameters  $B$  and  $C$  from Table 2.

The extrapolated values of  $Q$  are relatively insensitive to errors of the parameters  $B$  and  $C$ . As is shown by Eq. (5) the parameter  $B$  is equal to equimolar  $H^E$  at 298.15 K divided by the gas constant.  $B$  is more accurate than individual  $H^E$  measurements, because it is obtained from regression of many  $H^E$  points taken from various sources and compared in homologous series. From Eq. (6) one sees that the shift of  $Q$  caused by the shift of  $B$  is given by the formula:  $\Delta Q = \Delta B(1/T - 1/313.15)$ . Even if we overestimate the error of  $B$  assuming that  $\Delta B = 5$  K, then the corresponding shift of  $\Delta Q$  at the extrapolating distance  $T = 313 \pm 20$  K equals  $\Delta Q = 0.001$ . An error of  $Q$  obtained from good experimental VLE data is almost 1 order of magnitude higher. Hence we

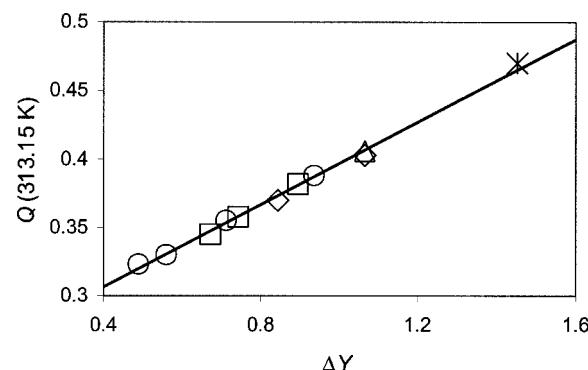


FIG. 2. Values of  $Q$  at 313.15 K for isomeric alkanols with benzene (circles), toluene (squares), xylenes (triangles), ethylbenzene (diamonds), and mesitilene (stars) plotted vs  $\Delta Y = (N_j + 1)^{0.5} - N_i^{0.5}$  and the line calculated with Eq. (7).

assume that an error of  $B$  has only a small influence on the calculated values of  $Q$  in the temperature range that occurred in this paper. It seems that the error of  $C$  is even less significant because  $C$  is almost constant and can be adjusted to  $H^E$  data or estimated with accuracy not less than 0.1.

For all the investigated mixtures both the correlation and prediction were done with parameters  $\Delta H_i/R$ ,  $K_{ii}$ , and  $\Delta b_i$  from Table 1.  $K_{ij}$  was calculated with Eq. (2) using  $\alpha=0.000\,80 \text{ MPa}^{-1}$ . In the case of correlation  $\Theta_{i,j}$  was adjusted to each data set individually, in the case of the prediction  $\Theta_{i,j}$  was calculated from the corresponding  $Q_{ij}$ . The resulting standard deviation of pressure ( $\sigma$ ) was calculated by Eq. (8)

$$\sigma = \left[ \sum_{k=1}^{N-n} (P_{\text{exper.}} - P_{\text{calc.}})_k^2 / (N-n-m) \right]^{0.5}, \quad (8)$$

where  $P_{\text{exper.}}$  is experimental pressure,  $P_{\text{calc.}}$  is calculated pressure,  $N$  is total number of the experimental points in the data set,  $n$  is the number of data points for pure substances, and  $m$  is number of the adjustable parameters. In the case of correlation  $m=1$ ; in the case of prediction  $m=0$  was used.

Both isothermal and isobaric data were treated in a uniform way in the respect that the vapor pressure and vapor composition were adjusted to liquid composition and temperature via EoS. Hence accuracy of the VLE description for both types of data is characterized by  $\sigma$  calculated with Eq. (8).

In the case of correlation  $\sigma$  depends mainly on scattering of the VLE data, whereas in the case of prediction,  $\sigma$  is additionally increased by systematic error of the data and error of the prediction. Thus the error of the prediction cannot be estimated from the corresponding  $\sigma$  alone. One should rather consider the difference between the standard deviations of the prediction and the correlation. The two values of  $\sigma$  corresponding to the prediction and the correlation are given below each data set. In order to summarize results for data sets measured at various conditions each  $\sigma$  was divided by the average pressure in the data set ( $\bar{P}$ ). The mean value of  $\sigma/\bar{P}$  for the recommended VLE data is 0.59% in the case of prediction and 0.51% for correlation. The small difference between these two values indicates excellent accuracy of the prediction as well as the absence of significant systematic errors in the recommended data.

#### 4. Description of Tables Containing the Recommended Data

Each system is presented on a separate page, which includes a table of VLE data, the corresponding figures, and auxiliary information. Each table is accompanied by two figures (pressure versus mole fraction and temperature versus mole fraction). In the tables and figures, subscript "1" for the component refers to the first chemical species listed under the subtitle "Components."

The verification procedure, described above, discarded more than half of the investigated data sets. For some sys-

tems, however, the remaining amount of data is still too large and must undergo further selection. In such cases the additional criteria described in Part 1<sup>1</sup> were used.

For many systems, however, there are not enough data to fill the corresponding table with the three isotherms and the isobaric data set. In such a case the table is completed with the predicted "artificial" data provided that at least one positively evaluated experimental data set is available for a given system. These artificial data sets are specified as "predicted." The value of  $Q$  used for the prediction is denoted as  $Q_0$  and given below each artificial data set.

Each experimental data set is accompanied by a  $Q$  value and standard deviation of pressure resulting from the correlation of the data with EoS. They are denoted by  $Q_1$  and  $\sigma_1$ , respectively. For comparison values of  $Q_0$  and  $\sigma_0$ , resulting from the prediction, are also given.

It was found that during the correlation of the isobaric data the temperature dependence of the binary parameter  $\Theta$  in EoS can be ignored, which reduces the number of adjustable parameters. As a consequence, isobaric data sets were correlated in a similar way as isothermal data using  $\Theta$  independent of temperature. In this case  $Q_0$  and  $Q_1$  given below the isobaric data set correspond to temperature at equimolar concentration of the data set.

If experimental vapor concentration  $y$  is not reported for the selected data set then the experimental data are appended with the calculated values of  $y$ . These values are not shown in the figures to differentiate them from the experimental points. The only points shown in the figures correspond to experimental values. The approximating lines result from correlation with EoS. For the artificial data sets only the predicted curves are shown.

#### 5. Conclusions

The whole collection of data sets for the 29 systems given in the paper is internally consistent, because separate data sets for various mixtures are approximated very well with the same Eq. (7). This statement is supported by the good agreement of  $Q_1$  and  $Q_0$  given below each experimental data set. The values of  $Q_1$  and  $Q_0$  describe the experimental data with similar accuracy, as is shown by values of the corresponding standard deviations  $\sigma_1$  and  $\sigma_0$ . The good accuracy of the prediction demonstrated on the experimental data suggests a corresponding good accuracy of the predicted data used to fill the experimental gaps in the tables.

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## 9. Appendix 2: Bibliography of $H^E$ Data for Alkanol–Aromatic Hydrocarbon Systems

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### 3. Recommended VLE Data for Alkanol–Aromatic Systems

Table 3.1. Methanol–benzene

Components		References		Reference vapor–liquid equilibrium data											
				T/K = 298.15, Ref. 1			T/K = 318.15, Ref. 2			T/K = 328.15, Ref. 3			P/kPa = 101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>				
12.71	0.0000	0.0000	29.894	0.0000	0.0000	62.11	0.0304	0.3019	353.22	0.00	0.0000				
19.00	0.0248	0.3275	32.744	0.0037	0.0882	70.28	0.0493	0.4051	338.62	0.05	0.3922				
20.83	0.0457	0.3970	35.358	0.0102	0.1567	79.66	0.1031	0.4841	335.13	0.10	0.4723				
21.78	0.0663	0.4311	38.587	0.0161	0.2364	88.56	0.3297	0.5540	333.69	0.15	0.5064				
23.10	0.1247	0.4747	40.962	0.0207	0.2794	90.08	0.4874	0.5845	332.93	0.20	0.5261				
23.92	0.2292	0.5042	44.231	0.0314	0.3391	90.12	0.4984	0.5858	332.47	0.25	0.5395				
24.34	0.3887	0.5272	46.832	0.0431	0.3794	90.45	0.6076	0.6078	332.17	0.30	0.5498				
24.43	0.4974	0.5414	50.488	0.0613	0.4306	88.65	0.7898	0.6716	331.95	0.35	0.5585				
24.43	0.5910	0.5563	53.224	0.0854	0.4642	82.96	0.9014	0.7697	331.79	0.40	0.5663				
24.25	0.6868	0.5780	55.571	0.1263	0.4921				331.67	0.45	0.5740				
23.85	0.7676	0.6066	57.454	0.1811	0.5171				331.59	0.50	0.5819				
23.10	0.8343	0.6451	58.427	0.2334	0.5288				331.53	0.55	0.5904				
21.81	0.8981	0.7088	59.402	0.3217	0.5450				331.51	0.60	0.6001				
19.83	0.9512	0.8084	59.802	0.3805	0.5538				331.54	0.65	0.6117				
16.92	1.0000	1.0000	60.015	0.4201	0.5590				331.62	0.70	0.6260				
			60.242	0.4746	0.5673				331.80	0.75	0.6445				
			60.416	0.5420	0.5783				332.12	0.80	0.6693				
			60.443	0.5716	0.5821				332.67	0.85	0.7044				
			60.416	0.6164	0.5908				333.61	0.90	0.7572				
			60.350	0.6509	0.5990				335.27	0.95	0.8430				
			60.215	0.6793	0.6067				338.33	1.00	1.0000				
			59.868	0.7259	0.6216										
			59.482	0.7575	0.6346										
			58.321	0.8171	0.6681										
			56.213	0.8744	0.7181										
			54.692	0.9033	0.7525										
			53.037	0.9264	0.7896										
			51.009	0.9497	0.8368										
			50.048	0.9594	0.8599										
			48.767	0.9707	0.8916										
			47.540	0.9804	0.9222										
			46.232	0.9895	0.9558										
			44.608	1.0000	1.0000										
$Q_1 = 0.509$		$\sigma_1 = 0.19 \text{ kPa}$		$Q_1 = 0.487$		$\sigma_1 = 0.31 \text{ kPa}$		$Q_1 = 0.480$		$\sigma_1 = 0.60 \text{ kPa}$		$Q_0 = 0.475$			
$Q_0 = 0.508$		$\sigma_0 = 0.19 \text{ kPa}$		$Q_0 = 0.489$		$\sigma_0 = 0.32 \text{ kPa}$		$Q_0 = 0.478$		$\sigma_0 = 0.59 \text{ kPa}$		$Q_0 = 0.475$			

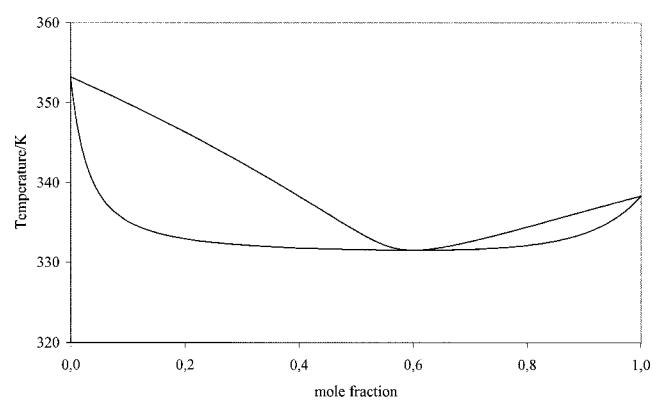
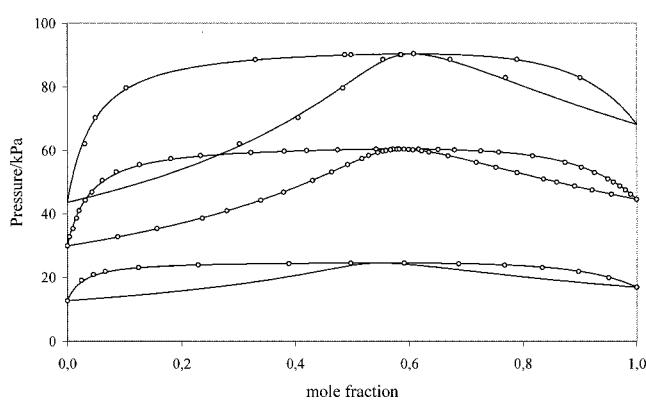


Table 3.2. Methanol–toluene

Components			References								
Methanol, CH <sub>4</sub> O [67-56-1]			<sup>1</sup> P. Oracz, G. Kolasinska, and B. Janaszewski (Unpublished data, Warsaw University, Warsaw, 1980).								
Reference vapor–liquid equilibrium data											
<i>T</i> /K=293.15, predicted		<i>T</i> /K=313.15, Ref. 1		<i>T</i> /K=333.15, predicted		<i>P</i> /kPa=101.32, predicted					
<i>P</i> /kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>P</i> /kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P</i> /kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>T</i> /K	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
2.91	0.00	0.0000	7.89	0.0000	0.0000	18.53	0.00	0.0000	383.89	0.00	0.0000
9.99	0.05	0.7162	20.18	0.0275	0.6209	53.68	0.05	0.6633	351.35	0.05	0.6504
11.47	0.10	0.7564	26.28	0.0589	0.7085	66.12	0.10	0.7320	344.59	0.10	0.7318
12.08	0.15	0.7710	29.20	0.0925	0.7420	72.25	0.15	0.7584	341.99	0.15	0.7605
12.41	0.20	0.7788	29.73	0.1011	0.7473	75.80	0.20	0.7727	340.66	0.20	0.7753
12.62	0.25	0.7838	32.28	0.1663	0.7707	78.09	0.25	0.7818	339.88	0.25	0.7844
12.76	0.30	0.7874	33.02	0.2007	0.7773	79.69	0.30	0.7883	339.36	0.30	0.7907
12.87	0.35	0.7904	34.42	0.2988	0.7887	80.88	0.35	0.7934	339.00	0.35	0.7957
12.95	0.40	0.7931	35.30	0.4188	0.7973	81.83	0.40	0.7979	338.72	0.40	0.7998
13.03	0.45	0.7958	36.23	0.5968	0.8103	82.64	0.45	0.8020	338.49	0.45	0.8036
13.11	0.50	0.7978	37.08	0.8045	0.8445	83.36	0.50	0.8061	338.29	0.50	0.8073
13.18	0.55	0.8020	37.18	0.8926	0.8812	84.05	0.55	0.8105	338.10	0.55	0.8113
13.26	0.60	0.8059	36.75	0.9485	0.9253	84.72	0.60	0.8154	337.92	0.60	0.8158
13.34	0.65	0.8108	36.25	0.9739	0.9561	85.38	0.65	0.8213	337.75	0.65	0.8212
13.41	0.70	0.8171	35.45	1.0000	1.0000	86.03	0.70	0.8286	337.57	0.70	0.8279
13.48	0.75	0.8254				86.66	0.75	0.8379	337.41	0.75	0.8367
13.55	0.80	0.8370				87.23	0.80	0.8503	337.26	0.80	0.8486
13.58	0.85	0.8538				87.64	0.85	0.8676	337.16	0.85	0.8654
13.55	0.90	0.8795				87.70	0.90	0.8929	337.16	0.90	0.8905
13.37	0.95	0.9219				87.04	0.95	0.9323	337.36	0.95	0.9303
12.88	1.00	1.0000				84.82	1.00	1.0000	338.05	1.00	1.0000
$Q_1 = 0.522$		$\sigma_1 = 0.15 \text{ kPa}$		$Q_0 = 0.540$		$\sigma_0 = 0.15 \text{ kPa}$		$Q_0 = 0.522$		$\sigma_0 = 0.15 \text{ kPa}$	
$Q_0 = 0.499$		$Q_0 = 0.493$									

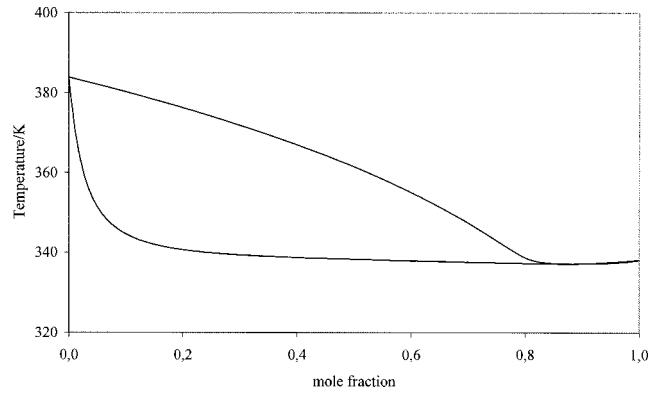
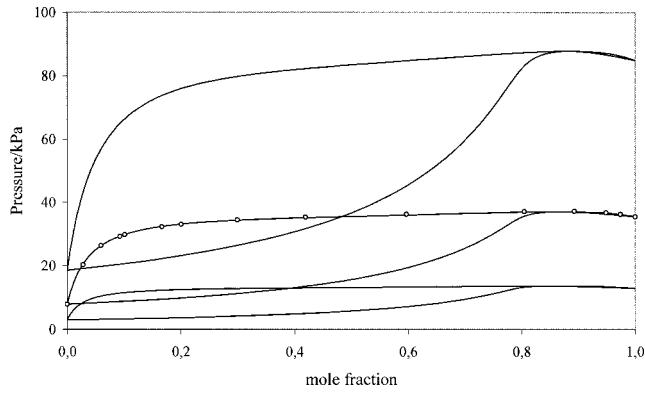


Table 3.3. Ethanol–benzene

<b>Components</b>		<b>References</b>									
Ethanol, C <sub>2</sub> H <sub>6</sub> O [64-17-5]		<sup>1</sup> J. Zielkiewicz, P. Oracz, and S. Warycha, Fluid Phase Equilib. <b>58</b> , 191 (1990).									
Benzene, C <sub>6</sub> H <sub>6</sub> [71-43-2]		<sup>2</sup> I. Brown and F. Smith, Aust. J. Chem. <b>7</b> , 264 (1954).									
		<sup>3</sup> V. V. Udovenko and L. G. Fatkulina, Zh. Fiz. Khim. <b>26</b> , 719 (1952).									
		<sup>4</sup> Q. Wang, G. Chen, and S. Han, Rantae Hwaxue Xuebae—J. Fuel Chem. Technol. <b>81</b> , 2 (1990).									
Reference vapor–liquid equilibrium data											
T/K = 303.15, Ref. 1			T/K = 318.15, Ref. 2			T/K = 333.15, Ref. 3			P/kPa = 101.30, Ref. 4		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
15.912	0.0000	0.0000	29.83	0.0000	0.0000	52.40	0.000	0.0000	353.26	0.0000	0.0000
19.900	0.0546	0.2223	36.13	0.0374	0.1965	60.35	0.026	0.1584	352.25	0.0029	0.0256
20.831	0.1239	0.2770	39.53	0.0972	0.2895	69.09	0.080	0.2755	349.79	0.0177	0.1070
21.169	0.2097	0.3044	40.87	0.2183	0.3370	73.82	0.185	0.3506	347.31	0.0440	0.1837
21.259	0.2757	0.3179	41.24	0.3141	0.3625	75.33	0.322	0.3945	343.65	0.1061	0.2973
21.264	0.3498	0.3308	41.28	0.4150	0.3842	75.73	0.398	0.4136	341.64	0.2124	0.3720
21.217	0.4070	0.3406	40.99	0.5199	0.4065	75.54	0.484	0.4357	340.97	0.3661	0.4252
21.047	0.4982	0.3580	40.93	0.5284	0.4101	75.01	0.568	0.4607	340.92	0.4641	0.4511
20.853	0.5539	0.3708	40.27	0.6155	0.4343	73.15	0.680	0.5053	340.97	0.5666	0.4836
20.799	0.5686	0.3746	38.90	0.7087	0.4751	69.89	0.771	0.5601	341.26	0.6394	0.5091
20.235	0.6583	0.4030	36.14	0.8102	0.5456	64.66	0.859	0.6462	342.34	0.7536	0.5753
19.793	0.7048	0.4229	30.36	0.9193	0.7078	57.54	0.929	0.7650	343.52	0.8095	0.6216
19.280	0.7449	0.4445	27.10	0.9591	0.8201	50.32	0.981	0.9177	346.33	0.9111	0.7555
17.967	0.8167	0.4991	23.05	1.0000	1.0000	47.14	1.000	1.0000	348.53	0.9570	0.8639
16.955	0.8562	0.5433							349.42	0.9729	0.9053
15.845	0.8911	0.5967							350.76	0.9907	0.9714
12.746	0.9619	0.7879							351.31	1.0000	1.0000
10.469	1.0000	1.0000									
$Q_1 = 0.446$	$\sigma_1 = 0.05 \text{ kPa}$		$Q_1 = 0.426$	$\sigma_1 = 0.12 \text{ kPa}$		$Q_1 = 0.406$	$\sigma_1 = 0.26 \text{ kPa}$		$Q_1 = 0.401$	$\sigma_1 = 0.89 \text{ kPa}$	
$Q_0 = 0.443$	$\sigma_0 = 0.07 \text{ kPa}$		$Q_0 = 0.425$	$\sigma_0 = 0.12 \text{ kPa}$		$Q_0 = 0.406$	$\sigma_0 = 0.25 \text{ kPa}$		$Q_0 = 0.395$	$\sigma_0 = 1.01 \text{ kPa}$	

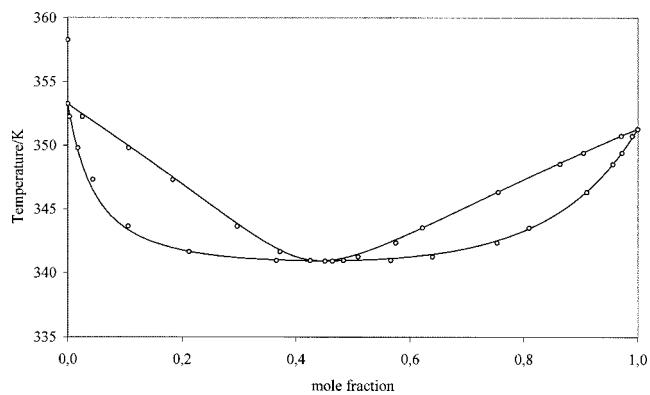
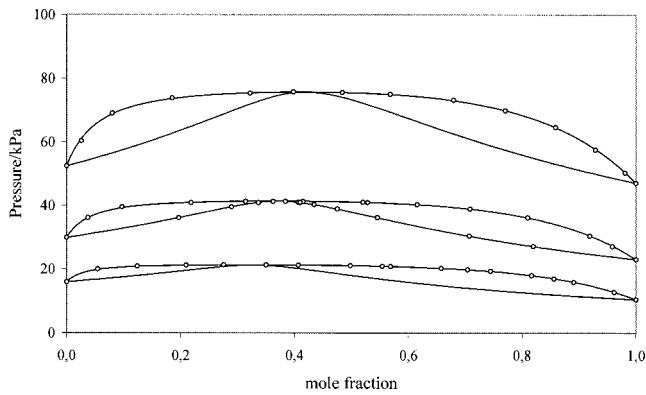


Table 3.4. Ethanol–toluene

Components		References		Reference vapor–liquid equilibrium data											
				T/K=308.15, Ref. 1			T/K=318.15, Ref. 2			T/K=328.15, Ref. 1			P/kPa=101.32, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>				
6.24	0.0000	0.0000	11.36	0.005	0.119	15.14	0.0000	0.0000	383.91	0.00	0.0000				
10.58	0.0330	0.4216	12.53	0.010	0.204	26.22	0.0439	0.4369	366.00	0.05	0.4344				
11.51	0.0468	0.4749	13.57	0.015	0.268	33.02	0.1157	0.5679	359.59	0.10	0.5537				
13.61	0.1214	0.5662	14.51	0.020	0.318	37.23	0.2497	0.6319	356.59	0.15	0.6058				
14.52	0.2079	0.6014	17.35	0.040	0.438	39.22	0.4034	0.6649	354.88	0.20	0.6356				
15.23	0.3620	0.6346	19.19	0.060	0.497	39.30	0.4142	0.6673	353.78	0.25	0.6558				
15.38	0.4160	0.6384	20.42	0.080	0.532	40.73	0.6282	0.7150	353.00	0.30	0.6710				
15.72	0.5930	0.6730	21.28	0.100	0.555	41.04	0.7186	0.7431	352.41	0.35	0.6836				
15.81	0.7263	0.7164	22.60	0.150	0.588	40.83	0.8423	0.8049	351.94	0.40	0.6948				
15.54	0.8519	0.7848	23.42	0.200	0.608	39.93	0.9163	0.8685	351.55	0.45	0.7053				
14.35	0.9701	0.9318	24.41	0.300	0.634	38.73	0.9635	0.9307	351.21	0.50	0.7158				
13.75	1.0000	1.0000	25.04	0.400	0.653	37.32	1.0000	1.0000	350.92	0.55	0.7266				
			25.50	0.500	0.672				350.67	0.60	0.7382				
			25.82	0.600	0.693				350.44	0.65	0.7513				
			25.98	0.700	0.719				350.26	0.70	0.7663				
			25.90	0.800	0.761				350.12	0.75	0.7843				
			25.67	0.850	0.794				350.06	0.80	0.8064				
			25.21	0.900	0.838				350.08	0.85	0.8346				
			24.40	0.950	0.902				350.26	0.90	0.8720				
									350.69	0.95	0.9239				
									351.51	1.00	1.0000				
$Q_1 = 0.463$	$\sigma_1 = 0.02 \text{ kPa}$	$Q_1 = 0.453$	$\sigma_1 = 0.09 \text{ kPa}$	$Q_1 = 0.438$	$\sigma_1 = 0.17 \text{ kPa}$										
$Q_0 = 0.465$	$\sigma_0 = 0.04 \text{ kPa}$	$Q_0 = 0.453$	$\sigma_0 = 0.09 \text{ kPa}$	$Q_0 = 0.440$	$\sigma_0 = 0.19 \text{ kPa}$									$Q_0 = 0.406$	

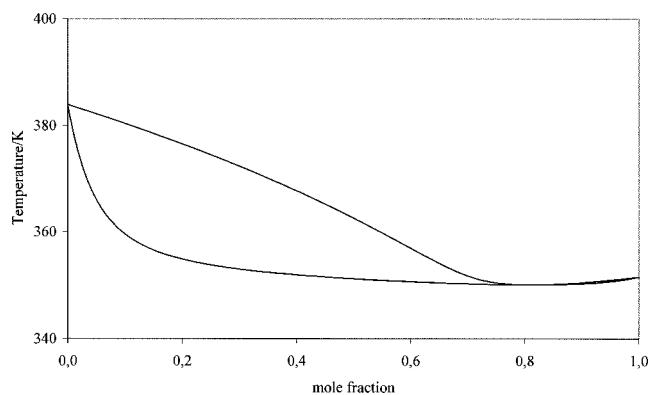
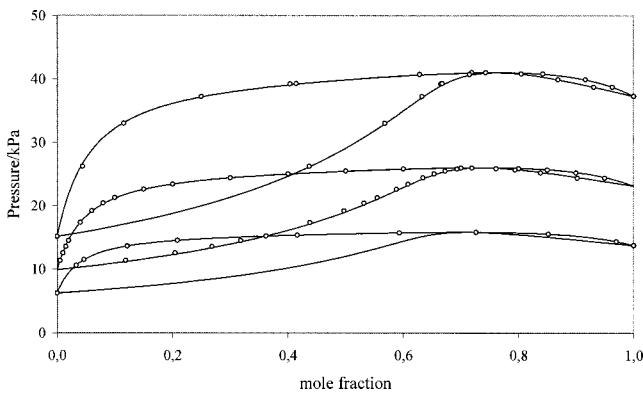


Table 3.5. Ethanol–1,4-dimethylbenzene

Components			References					
Ethanol, C <sub>2</sub> H <sub>6</sub> O [64-17-5]			<sup>1</sup> R. H. Stokes and H. T. French, J. Chem. Soc., Faraday Trans. 1, <b>76</b> , 537 (1980).					
1,4-Dimethylbenzene, C <sub>8</sub> H <sub>10</sub> [106-42-3]								
Reference vapor–liquid equilibrium data								
<i>T</i> /K = 318.15, Ref. 1		<i>T</i> /K = 338.15, predicted		<i>T</i> /K = 358.15, predicted		<i>P</i> /kPa = 101.32, predicted		
<i>P</i> /kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P</i> /kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>T</i> /K	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
4.446	0.00355	0.2577	8.52	0.00	0.0000	18.86	0.00	0.0000
4.954	0.00544	0.3395	27.91	0.05	0.7040	54.87	0.05	0.6653
5.464	0.00740	0.4041	36.25	0.10	0.7775	73.48	0.10	0.7562
5.926	0.00924	0.4517	40.85	0.15	0.8064	84.73	0.15	0.7931
7.125	0.01430	0.5425	43.78	0.20	0.8224	92.27	0.20	0.8138
7.614	0.01657	0.5712	45.82	0.25	0.8330	97.70	0.25	0.8274
8.518	0.02101	0.6146	47.36	0.30	0.8409	101.86	0.30	0.8375
10.061	0.02988	0.6711	48.60	0.35	0.8473	105.21	0.35	0.8456
11.284	0.03861	0.7059	49.63	0.40	0.8528	108.03	0.40	0.8525
12.280	0.04735	0.7299	50.55	0.45	0.8580	110.50	0.45	0.8587
13.527	0.06153	0.7562	51.38	0.50	0.8630	112.74	0.50	0.8647
14.459	0.07539	0.7734	52.17	0.55	0.8681	114.82	0.55	0.8706
15.164	0.08858	0.7853	52.94	0.60	0.8736	116.82	0.60	0.8768
15.740	0.10170	0.7944	53.69	0.65	0.8796	118.78	0.65	0.8835
16.216	0.11440	0.8014	54.45	0.70	0.8865	120.72	0.70	0.8909
16.944	0.13870	0.8117	55.22	0.75	0.8946	122.68	0.75	0.8995
17.500	0.16200	0.8190	56.00	0.80	0.9047	124.65	0.80	0.9099
17.932	0.18380	0.8244	56.78	0.85	0.9177	126.63	0.85	0.9229
18.428	0.21470	0.8305	57.52	0.90	0.9353	128.56	0.90	0.9400
18.904	0.25220	0.8363	58.15	0.95	0.9606	130.30	0.95	0.9640
19.262	0.28630	0.8407	58.44	1.00	1.0000	131.49	1.00	1.0000
19.542	0.31740	0.8441						
19.766	0.34610	0.8470						
19.954	0.37230	0.8495						
20.117	0.39690	0.8518						
20.260	0.41920	0.8538						
20.381	0.43970	0.8556						
20.484	0.45680	0.8571						
20.522	0.46820	0.8581						
20.761	0.51260	0.8620						
20.990	0.55790	0.8662						
21.200	0.59970	0.8704						
21.444	0.64760	0.8758						
21.694	0.69510	0.8820						
21.884	0.73100	0.8874						
22.086	0.76810	0.8939						
22.313	0.80910	0.9027						
22.501	0.84320	0.9116						
22.662	0.87240	0.9209						
22.761	0.89330	0.9288						
22.866	0.91500	0.9385						
22.950	0.93810	0.9507						
22.995	0.94990	0.9580						
23.037	0.96210	0.9664						
<i>Q</i> <sub>1</sub> = 0.475	<i>σ</i> <sub>1</sub> = 0.10 kPa		<i>Q</i> <sub>0</sub> = 0.452	<i>σ</i> <sub>0</sub> = 0.14 kPa		<i>Q</i> <sub>0</sub> = 0.421		
<i>Q</i> <sub>0</sub> = 0.479							<i>Q</i> <sub>0</sub> = 0.425	

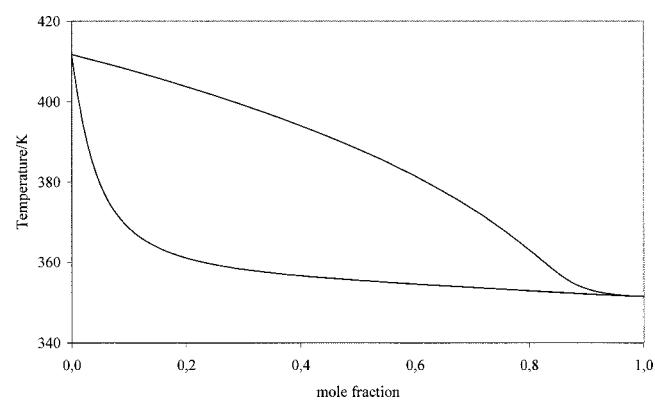
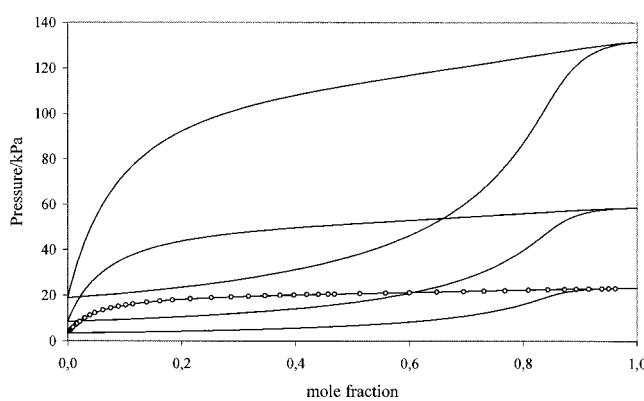


Table 3.6. 1-Propanol–benzene

Components			References								
1-Propanol, C <sub>3</sub> H <sub>8</sub> O [71-23-8]			<sup>1</sup> J. M. Rhodes, T. A. Griffin, M. J. Lazzaroni, V. R. Bhethanabotla, and S. W. Campbell, Fluid Phase Equilib. <b>179</b> , 217 (2001).								
Benzene, C <sub>6</sub> H <sub>6</sub> [71-43-2]			<sup>2</sup> K. Kurihara, M. Uchiyama, and K. Kojima, J. Chem. Eng. Data <b>42</b> , 149 (1997).								
			<sup>3</sup> S. J. Fu and B. C.-Y. Lu, J. Appl. Chem. <b>16</b> , 324 (1966).								
			<sup>4</sup> T. Hiaki, K. Tochigi, and K. Kojima, Fluid Phase Equilib. <b>26</b> , 83 (1986).								
Reference vapor–liquid equilibrium data											
T/K=313.15, Ref. 1			T/K=333.15, Ref. 2			T/K=348.15, Ref. 3			P/kPa=101.325, Ref. 4		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
24.541	0.0000	0.0000	55.43	0.050	0.094	90.43	0.0376	0.0768	351.74	0.031	0.070
25.554	0.0295	0.0606	55.84	0.066	0.110	93.71	0.0920	0.1435	350.47	0.101	0.157
25.931	0.0598	0.0907	55.91	0.068	0.111	94.15	0.0984	0.1490	350.14	0.135	0.180
26.069	0.0997	0.1133	55.96	0.072	0.115	95.27	0.2048	0.2085	350.09	0.194	0.202
26.043	0.1500	0.1309	56.13	0.081	0.122	94.77	0.2344	0.2145	350.07	0.200	0.204
25.942	0.1999	0.1433	56.24	0.087	0.127	94.43	0.3092	0.2420	350.06	0.203	0.205
25.778	0.2502	0.1534	56.28	0.091	0.130	93.05	0.4172	0.2797	350.07	0.213	0.209
25.583	0.3001	0.1623	56.37	0.096	0.134	88.53	0.5390	0.3185	350.06	0.219	0.208
25.334	0.3505	0.1709	56.52	0.111	0.143	84.59	0.6340	0.3494	350.06	0.221	0.211
25.049	0.4003	0.1794	56.62	0.126	0.151	77.37	0.7440	0.4225	350.07	0.232	0.214
24.697	0.4504	0.1885	56.67	0.142	0.157	67.47	0.8395	0.5265	350.11	0.247	0.217
24.219	0.5003	0.1984	56.70	0.157	0.163	55.04	0.9190	0.6868	350.20	0.296	0.230
24.219	0.5004	0.1985	56.70	0.179	0.172	50.88	0.9495	0.7695	350.30	0.317	0.236
24.273	0.5004	0.1985	56.68	0.197	0.180				350.36	0.337	0.244
23.686	0.5504	0.2098	56.61	0.217	0.186				350.47	0.358	0.252
23.030	0.6005	0.2231	56.55	0.235	0.191				350.66	0.396	0.265
22.214	0.6506	0.2393	56.22	0.303	0.207				350.76	0.419	0.269
21.206	0.7007	0.2597	55.83	0.344	0.218				350.78	0.433	0.275
19.913	0.7509	0.2864	55.46	0.377	0.225				351.69	0.521	0.311
18.308	0.8008	0.3229	55.19	0.397	0.230				353.00	0.630	0.368
16.300	0.8502	0.3754	54.96	0.416	0.234				355.46	0.733	0.437
13.828	0.9007	0.4612	54.71	0.433	0.239				357.02	0.784	0.486
11.418	0.9407	0.5776	53.53	0.490	0.254				361.87	0.896	0.660
9.358	0.9705	0.7261	52.75	0.543	0.266						
7.047	1.0000	1.0000	52.41	0.552	0.270						
			50.91	0.608	0.287						
			50.56	0.618	0.294						
			47.23	0.694	0.334						
			45.92	0.730	0.352						
			44.43	0.758	0.373						
			43.03	0.781	0.391						
			37.59	0.856	0.477						
			36.16	0.869	0.507						
			28.61	0.943	0.679						
Q <sub>1</sub> =0.382	σ <sub>1</sub> =0.06 kPa	Q <sub>1</sub> =0.356	σ <sub>1</sub> =0.13 kPa	Q <sub>1</sub> =0.322	σ <sub>1</sub> =0.56 kPa	Q <sub>1</sub> =0.315	σ <sub>1</sub> =0.34 kPa				
Q <sub>0</sub> =0.384	σ <sub>0</sub> =0.06 kPa	Q <sub>0</sub> =0.353	σ <sub>0</sub> =0.18 kPa	Q <sub>0</sub> =0.328	σ <sub>0</sub> =0.71 kPa	Q <sub>0</sub> =0.322	σ <sub>0</sub> =0.68 kPa				

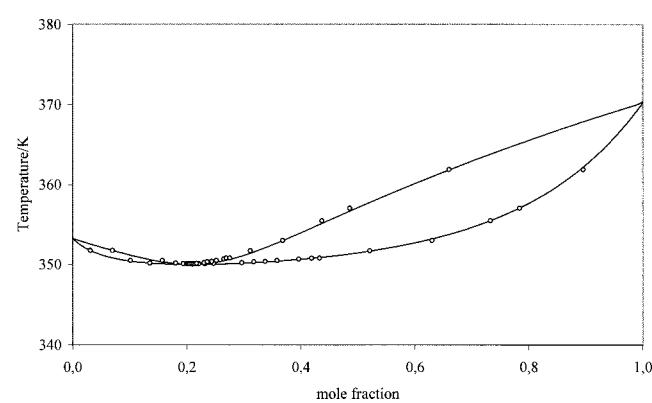
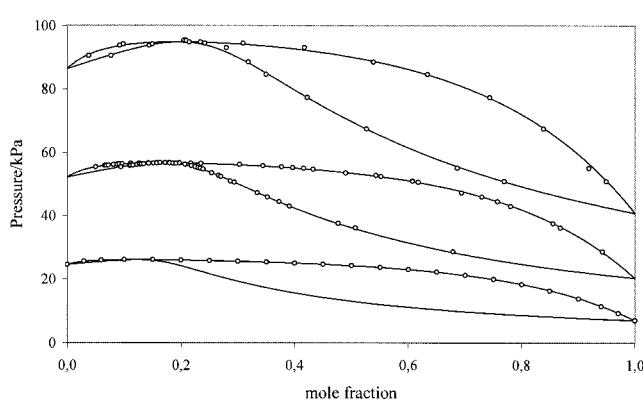


Table 3.7. 1-Propanol-toluene

Components			References								
1-Propanol, C <sub>3</sub> H <sub>8</sub> O [71-23-8]			<sup>1</sup> P. Oracz and G. Kolasinska, Fluid Phase Equilib. <b>35</b> , 253 (1987).								
Toluene, C <sub>7</sub> H <sub>8</sub> [108-88-3]			<sup>2</sup> B. C.-Y. Lu, Can. J. Technol. <b>34</b> , 468 (1957).								
Reference vapor-liquid equilibrium data											
<i>T</i> /K=313.15, Ref. 1		<i>T</i> /K=333.15, predicted		<i>T</i> /K=353.15, predicted							
<i>P</i> /kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P</i> /kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>P</i> /kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>T</i> /K	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>
7.89	0.0000	0.0000	18.53	0.00	0.0000	38.84	0.00	0.0000	377.25	0.046	0.211
9.21	0.0268	0.1632	23.23	0.05	0.2324	48.46	0.05	0.2293	371.55	0.121	0.366
10.17	0.0659	0.2544	25.30	0.10	0.3154	53.55	0.10	0.3250	369.45	0.188	0.440
10.27	0.0717	0.2627	26.45	0.15	0.3609	56.67	0.15	0.3800	367.35	0.268	0.482
11.00	0.1554	0.3332	27.16	0.20	0.3915	58.75	0.20	0.4177	366.55	0.444	0.556
11.11	0.1945	0.3519	27.64	0.25	0.4148	60.22	0.25	0.4464	365.95	0.571	0.603
11.28	0.2809	0.3824	27.98	0.30	0.4342	61.31	0.30	0.4701	365.75	0.600	0.617
11.33	0.3337	0.3977	28.21	0.35	0.4515	62.13	0.35	0.4909	366.05	0.762	0.699
11.35	0.4031	0.4163	28.37	0.40	0.4676	62.75	0.40	0.5101	366.65	0.804	0.728
11.34	0.4622	0.4320	28.46	0.45	0.4834	63.20	0.45	0.5286	367.05	0.858	0.786
11.28	0.5341	0.4523	28.49	0.50	0.4994	63.50	0.50	0.5471	368.65	0.940	0.897
11.16	0.6033	0.4746	28.46	0.55	0.5163	63.65	0.55	0.5662	368.95	0.961	0.921
10.98	0.6687	0.5001	28.35	0.60	0.5346	63.66	0.60	0.5865			
10.73	0.7299	0.5304	28.16	0.65	0.5553	63.49	0.65	0.6088			
10.30	0.7937	0.5730	27.86	0.70	0.5793	63.12	0.70	0.6341			
10.19	0.8106	0.5871	27.42	0.75	0.6082	62.48	0.75	0.6637			
9.88	0.8400	0.6156	26.79	0.80	0.6443	61.50	0.80	0.6994			
9.07	0.9029	0.7015	25.90	0.85	0.6913	60.06	0.85	0.7441			
8.83	0.9192	0.7322	24.64	0.90	0.7557	58.00	0.90	0.8024			
8.63	0.9305	0.7566	22.87	0.95	0.8497	55.07	0.95	0.8825			
7.01	1.0000	1.0000	20.36	1.00	1.0000	50.92	1.00	1.0000			
<i>Q</i> <sub>1</sub> =0.410		$\sigma_1=0.06 \text{ kPa}$							<i>Q</i> <sub>1</sub> =0.327		$\sigma_1=0.80 \text{ kPa}$
<i>Q</i> <sub>0</sub> =0.411		$\sigma_0=0.06 \text{ kPa}$		<i>Q</i> <sub>0</sub> =0.381				<i>Q</i> <sub>0</sub> =0.347		<i>Q</i> <sub>0</sub> =0.323	$\sigma_0=5 \text{ kPa}$

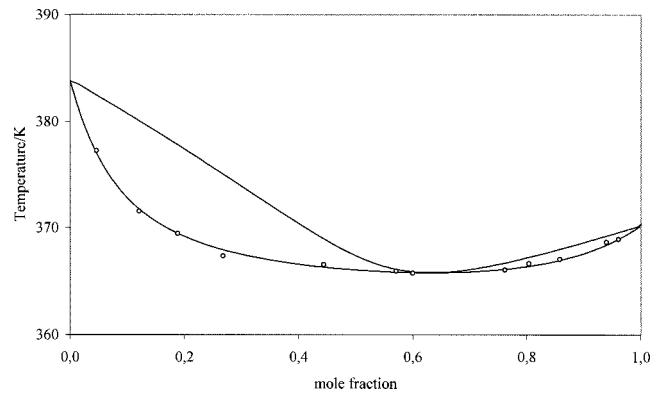
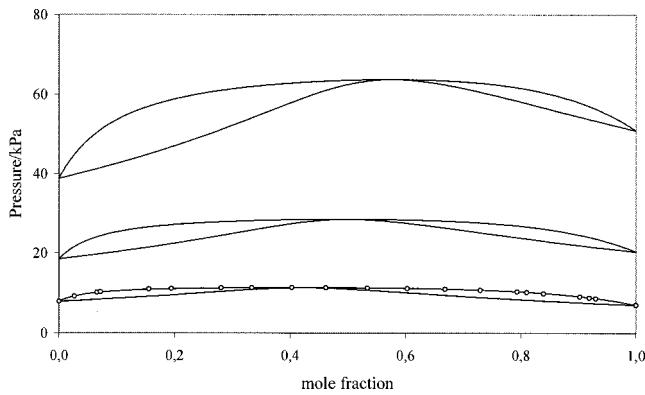


Table 3.8. 1-Propanol–1,4-dimethylbenzene

Components			References								
1-Propanol, C <sub>3</sub> H <sub>8</sub> O [71-23-8]			<sup>1</sup> P. Oracz and G. Kolasinska, Int. DATA Ser., Sel. Data Mixtures, Ser. A <b>24</b> , 277 (1996).								
1,4-Dimethylbenzene, C <sub>8</sub> H <sub>10</sub> [106-42-3]			<sup>2</sup> A. Galska-Krajewska, Roczn. Chem. <b>41</b> , 609 (1967).								
Reference vapor–liquid equilibrium data											
<i>T/K</i> =313.15, Ref. 1		<i>T/K</i> =333.15, predicted		<i>T/K</i> =353.15, predicted							
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>T/K</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
2.652	0.0000	0.0000	6.87	0.00	0.0000	15.66	0.00	0.0000	411.52	0.000	0.000
5.300	0.0689	0.5179	12.29	0.05	0.4613	26.72	0.05	0.4358	398.42	0.040	0.326
6.199	0.1439	0.6002	14.84	0.10	0.5667	32.90	0.10	0.5562	392.42	0.070	0.445
6.846	0.2636	0.6527	16.35	0.15	0.6162	36.88	0.15	0.6150	383.49	0.141	0.611
6.966	0.3156	0.6675	17.36	0.20	0.6466	39.68	0.20	0.6514	379.50	0.211	0.670
7.087	0.3763	0.6824	18.11	0.25	0.6682	41.79	0.25	0.6772	374.63	0.428	0.744
7.119	0.3931	0.6863	18.69	0.30	0.6852	43.46	0.30	0.6972	373.16	0.508	0.774
7.179	0.4396	0.6965	19.16	0.35	0.6995	44.83	0.35	0.7139	372.50	0.569	0.790
7.253	0.4834	0.7060	19.55	0.40	0.7122	45.99	0.40	0.7284	372.00	0.627	0.804
7.322	0.5296	0.7160	19.89	0.45	0.7240	47.00	0.45	0.7418	371.99	0.645	0.810
7.365	0.5629	0.7233	20.19	0.50	0.7353	47.88	0.50	0.7544	371.07	0.732	0.837
7.415	0.5956	0.7309	20.45	0.55	0.7466	48.67	0.55	0.7669	370.51	0.811	0.867
7.446	0.6252	0.7380	20.68	0.60	0.7583	49.39	0.60	0.7796	370.21	0.863	0.894
7.498	0.6899	0.7554	20.88	0.65	0.7709	50.03	0.65	0.7929	370.04	0.922	0.929
7.529	0.7532	0.7763	21.06	0.70	0.7849	50.61	0.70	0.8075	370.05	0.938	0.940
7.539	0.7991	0.7953	21.20	0.75	0.8012	51.13	0.75	0.8240	370.05	0.948	0.949
7.494	0.8729	0.8378	21.30	0.80	0.8209	51.55	0.80	0.8435	370.05	0.949	0.950
7.378	0.9262	0.8849	21.32	0.85	0.8460	51.84	0.85	0.8673	370.03	0.952	0.953
7.006	1.0000	1.0000	21.24	0.90	0.8795	51.94	0.90	0.8980	370.03	0.954	0.954
			20.96	0.95	0.9272	51.71	0.95	0.9397	370.04	0.970	0.969
			20.35	1.00	1.0000	50.89	1.00	1.0000	370.04	0.971	0.970
									370.04	0.972	0.970
									370.04	0.976	0.975
									370.07	0.985	0.983
									370.12	1.000	1.000
<i>Q</i> <sub>1</sub> =0.431	$\sigma_1=0.05 \text{ kPa}$		<i>Q</i> <sub>0</sub> =0.437	$\sigma_0=0.07 \text{ kPa}$		<i>Q</i> <sub>0</sub> =0.406	<i>Q</i> <sub>0</sub> =0.372		<i>Q</i> <sub>1</sub> =0.338	$\sigma_1=1.13 \text{ kPa}$	
									<i>Q</i> <sub>0</sub> =0.335	$\sigma_0=1.13 \text{ kPa}$	

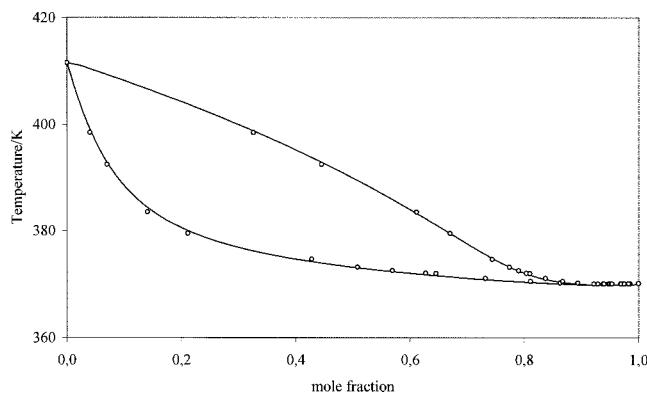
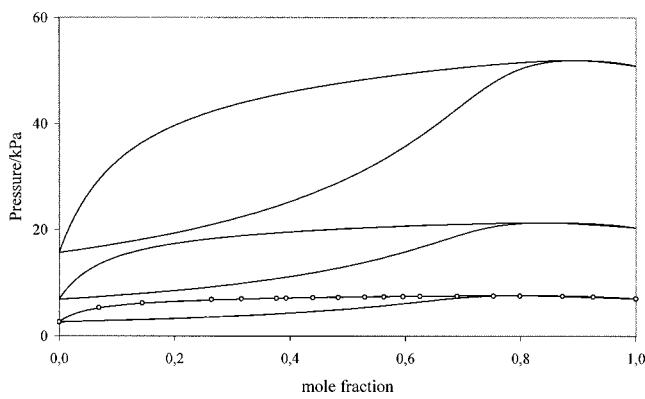


Table 3.9. 1-Propanol–ethylbenzene

Components			References								
1-Propanol, C <sub>3</sub> H <sub>8</sub> O [71-23-8]			'S. R. M. Ellis and B. A. Froome, Chem. Ind. Rev. 237 (1954).								
Ethylbenzene, C <sub>8</sub> H <sub>10</sub> [100-41-4]											
Reference vapor–liquid equilibrium data											
<i>T/K</i> =313.15, predicted			<i>T/K</i> =333.15, predicted								
<i>P/kPa</i>	<i>x<sub>1</sub></i>	<i>y<sub>1</sub></i>	<i>P/kPa</i>	<i>x<sub>1</sub></i>	<i>y<sub>1</sub></i>	<i>P/kPa</i>	<i>x<sub>1</sub></i>	<i>y<sub>1</sub></i>	<i>T/K</i>	<i>x<sub>1</sub></i>	<i>y<sub>1</sub></i>
2.87	0.00	0.0000	7.40	0.00	0.0000	16.77	0.00	0.0000	392.05	0.067	0.413
5.11	0.05	0.4590	12.78	0.05	0.4426	27.72	0.05	0.4176	389.45	0.087	0.466
5.96	0.10	0.5480	15.30	0.10	0.5479	33.82	0.10	0.5375	386.45	0.116	0.527
6.43	0.15	0.5891	16.79	0.15	0.5978	37.73	0.15	0.5969	383.35	0.144	0.584
6.73	0.20	0.6145	17.78	0.20	0.6286	40.47	0.20	0.6339	381.55	0.176	0.609
6.94	0.25	0.6329	18.51	0.25	0.6507	42.54	0.25	0.6603	378.95	0.224	0.655
7.11	0.30	0.6476	19.07	0.30	0.6681	44.17	0.30	0.6809	377.15	0.277	0.683
7.24	0.35	0.6602	19.53	0.35	0.6827	45.50	0.35	0.6981	375.95	0.320	0.701
7.35	0.40	0.6716	19.91	0.40	0.6958	46.63	0.40	0.7132	374.95	0.372	0.720
7.44	0.45	0.6823	20.24	0.45	0.7079	47.61	0.45	0.7271	374.05	0.425	0.735
7.52	0.50	0.6928	20.52	0.50	0.7196	48.46	0.50	0.7403	373.15	0.495	0.755
7.58	0.55	0.7035	20.76	0.55	0.7314	49.22	0.55	0.7534	372.55	0.544	0.768
7.64	0.60	0.7148	20.98	0.60	0.7436	49.91	0.60	0.7668	371.95	0.599	0.783
7.69	0.65	0.7272	21.17	0.65	0.7568	50.52	0.65	0.7809	371.45	0.664	0.802
7.72	0.70	0.7414	21.32	0.70	0.7716	51.06	0.70	0.7964	371.15	0.714	0.819
7.74	0.75	0.7583	21.44	0.75	0.7888	51.52	0.75	0.8139	370.75	0.759	0.835
7.73	0.80	0.7796	21.51	0.80	0.8098	51.88	0.80	0.8346	370.75	0.771	0.841
7.68	0.85	0.8077	21.49	0.85	0.8365	52.10	0.85	0.8600	370.35	0.867	0.889
7.58	0.90	0.8468	21.35	0.90	0.8722	52.10	0.90	0.8926	370.25	0.912	0.920
7.37	0.95	0.9052	21.01	0.95	0.9228	51.73	0.95	0.9366	370.15	0.942	0.944
6.99	1.00	1.0000	20.30	1.00	1.0000	50.76	1.00	1.0000			
<i>Q<sub>0</sub></i> =0.437			<i>Q<sub>0</sub></i> =0.405			<i>Q<sub>0</sub></i> =0.370			<i>Q<sub>1</sub></i> =0.330	<i>σ<sub>1</sub></i> =0.60 kPa	
						<i>Q<sub>0</sub></i> =0.331			<i>Q<sub>0</sub></i> =0.331	<i>σ<sub>0</sub></i> =0.60 kPa	

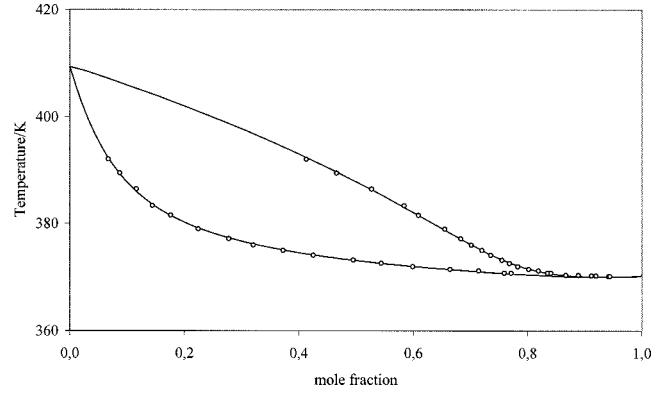
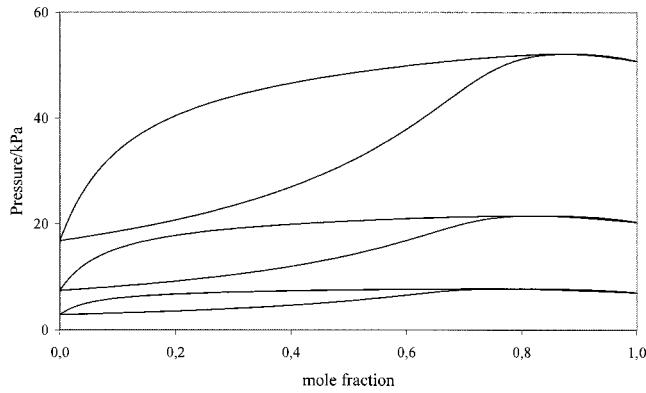


Table 3.10. 1-Butanol–benzene

Components			References								
1-Butanol, C <sub>4</sub> H <sub>10</sub> O [71-36-3]	<sup>1</sup> B. B. Allen, S. P. Lingo, and W. A. Felsing, J. Phys. Chem. <b>43</b> , 425 (1939).										
Benzene, C <sub>6</sub> H <sub>6</sub> [71-43-2]	<sup>2</sup> I. Brown and F. Smith, Aust. J. Chem. <b>12</b> , 407 (1959).										
Reference vapor–liquid equilibrium data											
<i>T/K</i> =298.15, Ref. 1		<i>T/K</i> =318.15, Ref. 2		<i>T/K</i> =338.15, predicted							
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>T/K</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
12.59	0.000	0.0000	29.82	0.0000	0.0000	62.14	0.00	0.0000	353.19	0.00	0.0000
11.91	0.197	0.0355	29.50	0.0538	0.0323	61.88	0.05	0.0366	353.16	0.05	0.0434
11.44	0.313	0.0421	29.18	0.0974	0.0432	61.17	0.10	0.0559	353.43	0.10	0.0693
10.39	0.500	0.0537	28.37	0.1986	0.0579	60.33	0.15	0.0689	353.82	0.15	0.0883
8.99	0.650	0.0692	27.42	0.3007	0.0684	59.42	0.20	0.0792	354.29	0.20	0.1042
6.88	0.798	0.1042	26.31	0.4004	0.0779	58.44	0.25	0.0881	354.83	0.25	0.1186
0.85	1.000	1.0000	25.01	0.4915	0.0885	57.37	0.30	0.0964	355.44	0.30	0.1326
			22.84	0.6003	0.1054	56.19	0.35	0.1045	356.15	0.35	0.1469
			19.84	0.7072	0.1311	54.88	0.40	0.1130	356.96	0.40	0.1621
			15.20	0.8206	0.1893	53.40	0.45	0.1220	357.89	0.45	0.1788
			3.38	1.0000	1.0000	51.72	0.50	0.1321	358.99	0.50	0.1977
						49.79	0.55	0.1435	360.26	0.55	0.2197
						47.57	0.60	0.1570	361.77	0.60	0.2457
						45.01	0.65	0.1733	363.55	0.65	0.2774
						42.03	0.70	0.1938	365.66	0.70	0.3168
						38.58	0.75	0.2207	368.17	0.75	0.3667
						34.56	0.80	0.2574	371.16	0.80	0.4314
						29.87	0.85	0.3114	374.71	0.85	0.5169
						24.42	0.90	0.3986	378.92	0.90	0.6317
						18.07	0.95	0.5641	383.84	0.95	0.7875
						10.68	1.00	1.0000	389.51	1.00	1.0000
<i>Q</i> <sub>1</sub> =0.362	<i>σ</i> <sub>1</sub> =0.07 kPa	<i>Q</i> <sub>1</sub> =0.338	<i>σ</i> <sub>1</sub> =0.006 kPa								
<i>Q</i> <sub>0</sub> =0.366	<i>σ</i> <sub>0</sub> =0.07 kPa	<i>Q</i> <sub>0</sub> =0.335	<i>σ</i> <sub>0</sub> =0.08 kPa								
								<i>Q</i> <sub>0</sub> =0.302			<i>Q</i> <sub>0</sub> =0.265

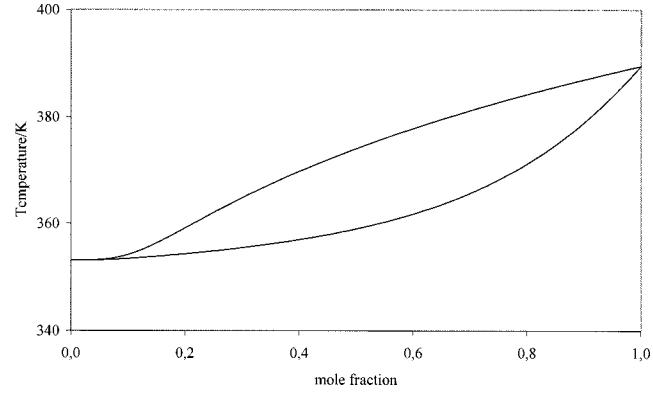
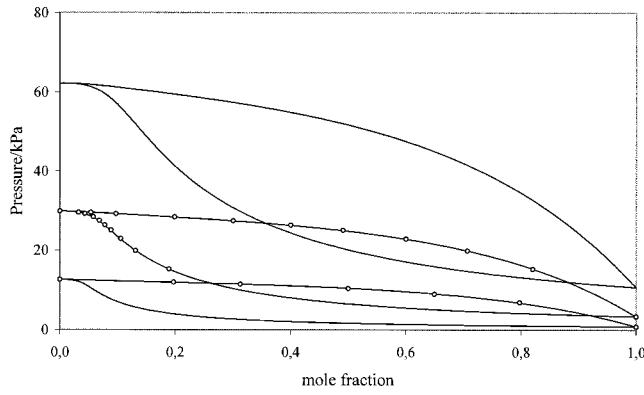


Table 3.11. 1-Butanol–toluene

<b>Components</b>		<b>References</b>						
1-Butanol, C <sub>4</sub> H <sub>10</sub> O [71-36-3]		<sup>1</sup> J. Lnenickova and I. Wichterle, Collect. Czech. Chem. Commun. <b>42</b> , 1907 (1977).						
Toluene, C <sub>7</sub> H <sub>8</sub> [108-88-3]		<sup>2</sup> A. N. Gorbunov, M. P. Susarev, and I. M. Balashova, Zh. Prikl. Khim. (Leningrad) <b>41</b> , 312 (1968).						
		<sup>3</sup> R. S. Mann and L. W. Shemilt, J. Chem. Eng. Data <b>8</b> , 189 (1963).						
Reference vapor–liquid equilibrium data								
<i>T/K</i> =333.31, Ref. 1		<i>T/K</i> =353.44, Ref. 1		<i>T/K</i> =373.15, Ref. 2		<i>P/kPa</i> =101.32, Ref. 3		
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>T/K</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
18.64	0.000	0.000	39.22	0.000	0.000	74.13	0.0	0.000
19.20	0.019	0.043	40.30	0.018	0.042	81.95	0.1	0.170
19.94	0.060	0.104	42.12	0.060	0.111	84.90	0.2	0.242
20.18	0.086	0.131	43.57	0.140	0.191	85.49	0.3	0.306
20.46	0.141	0.164	44.06	0.202	0.225	85.10	0.4	0.355
20.51	0.204	0.192	44.11	0.295	0.255	83.23	0.5	0.410
20.33	0.316	0.227	42.98	0.487	0.336	81.94	0.6	0.455
19.95	0.416	0.254	41.95	0.548	0.362	78.29	0.7	0.524
19.50	0.498	0.277	40.89	0.611	0.391	72.42	0.8	0.602
18.45	0.613	0.325	40.07	0.651	0.414	64.58	0.9	0.750
17.87	0.663	0.348	39.08	0.691	0.436	52.80	1.0	1.000
16.26	0.760	0.408	35.11	0.806	0.536			
13.70	0.866	0.533	31.31	0.883	0.645			
12.97	0.889	0.574	28.47	0.927	0.739			
9.75	0.969	0.815	25.40	0.967	0.852			
8.76	0.990	0.927	23.42	0.989	0.944			
8.22	1.000	1.000	22.40	1.000	1.000			
<i>Q</i> <sub>1</sub> =0.342		<i>σ</i> <sub>1</sub> =0.10 kPa	<i>Q</i> <sub>1</sub> =0.307		<i>σ</i> <sub>1</sub> =0.11 kPa	<i>Q</i> <sub>1</sub> =0.266		<i>σ</i> <sub>1</sub> =0.30 kPa
<i>Q</i> <sub>0</sub> =0.340		<i>σ</i> <sub>0</sub> =0.10 kPa	<i>Q</i> <sub>0</sub> =0.306		<i>σ</i> <sub>0</sub> =0.11 kPa	<i>Q</i> <sub>0</sub> =0.271		<i>σ</i> <sub>0</sub> =0.46 kPa
<i>Q</i> <sub>1</sub> =0.255		<i>σ</i> <sub>1</sub> =0.39 kPa	<i>Q</i> <sub>0</sub> =0.260		<i>σ</i> <sub>0</sub> =0.54 kPa			

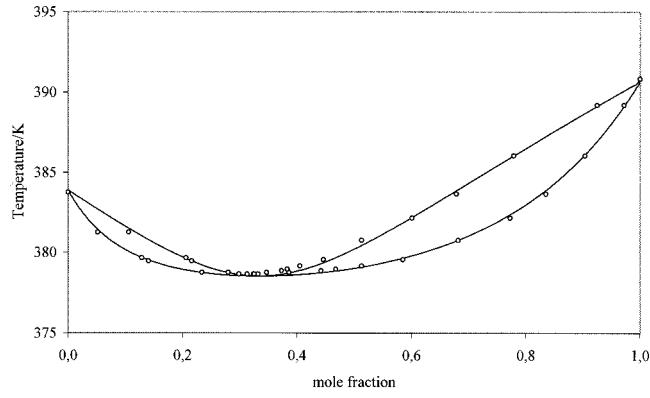
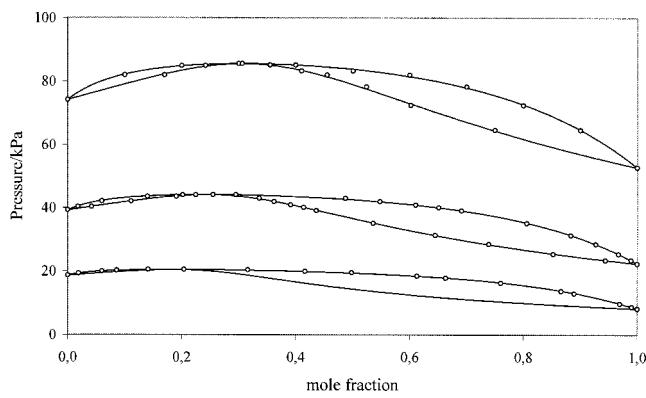


Table 3.12. 1-Butanol–1,4-dimethylbenzene

Components			References		
1-Butanol, C <sub>4</sub> H <sub>10</sub> O [71-36-3]			<sup>1</sup> P. Oracz and G. Kolasinska, Int. DATA Ser., Sel. Data Mixtures, Ser. A <b>24</b> , 286 (1996).		
1,4-Dimethylbenzene, C <sub>8</sub> H <sub>10</sub> [106-42-3]					
Reference vapor–liquid equilibrium data					
<i>T/K</i> =313.15, Ref. 1		<i>T/K</i> =333.15, predicted		<i>T/K</i> =353.15, predicted	
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
2.652	0.0000	0.0000	6.87	0.00	0.0000
3.086	0.0240	0.1479	8.64	0.05	0.2359
3.304	0.0473	0.2166	9.47	0.10	0.3237
3.530	0.0964	0.2904	9.95	0.15	0.3737
3.637	0.1304	0.3204	10.27	0.20	0.4082
3.737	0.1916	0.3579	10.50	0.25	0.4351
3.768	0.2128	0.3681	10.67	0.30	0.4576
3.830	0.2917	0.3999	10.79	0.35	0.4775
3.853	0.3823	0.4299	10.88	0.40	0.4959
3.869	0.4195	0.4413	10.94	0.45	0.5136
3.818	0.5699	0.4881	10.98	0.50	0.5310
3.794	0.6423	0.5144	10.99	0.55	0.5489
3.793	0.6470	0.5163	10.98	0.60	0.5677
3.593	0.7812	0.5868	10.93	0.65	0.5885
3.522	0.8040	0.6039	10.85	0.70	0.6120
3.356	0.8557	0.6533	10.72	0.75	0.6398
2.794	0.9647	0.8592	10.53	0.80	0.6739
2.516	1.0000	1.0000	10.25	0.85	0.7179
			9.83	0.90	0.7776
			9.24	0.95	0.8639
			8.36	1.00	1.0000

<i>Q</i> <sub>1</sub> =0.397	$\sigma_1=0.03 \text{ kPa}$	<i>Q</i> <sub>0</sub> =0.397	$\sigma_0=0.03 \text{ kPa}$	<i>Q</i> <sub>0</sub> =0.367	<i>Q</i> <sub>0</sub> =0.334	<i>Q</i> <sub>0</sub> =0.69
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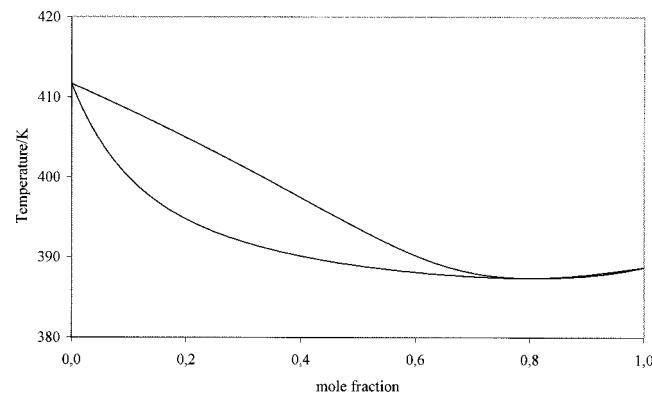
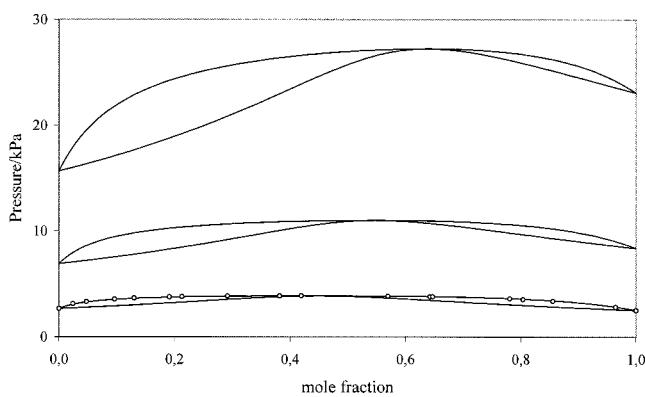


Table 3.13. 1-Butanol–ethylbenzene

Components			References					
1-Butanol, C <sub>4</sub> H <sub>10</sub> O [71-36-3]			<sup>1</sup> S. R. M. Ellis and M. Razavipour, Chem. Eng. Sci. <b>11</b> , 99 (1959).					
Ethylbenzene, C <sub>8</sub> H <sub>10</sub> [100-41-4]			Reference vapor–liquid equilibrium data					
<i>T/K</i> =313.15, predicted			<i>T/K</i> =333.15, predicted			<i>T/K</i> =353.15, predicted		
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
2.86	0.00	0.0000	7.41	0.00	0.0000	16.81	0.00	0.0000
3.44	0.05	0.1991	9.03	0.05	0.2113	20.46	0.05	0.2121
3.66	0.10	0.2656	9.77	0.10	0.2933	22.46	0.10	0.3066
3.77	0.15	0.3031	10.20	0.15	0.3408	23.73	0.15	0.3635
3.84	0.20	0.3295	10.48	0.20	0.3741	24.60	0.20	0.4038
3.88	0.25	0.3505	10.67	0.25	0.4002	25.24	0.25	0.4353
3.90	0.30	0.3685	10.80	0.30	0.4223	25.72	0.30	0.4617
3.92	0.35	0.3846	10.89	0.35	0.4420	26.08	0.35	0.4851
3.92	0.40	0.3998	10.96	0.40	0.4603	26.36	0.40	0.5066
3.92	0.45	0.4146	10.99	0.45	0.4779	26.56	0.45	0.5272
3.90	0.50	0.4297	11.00	0.50	0.4955	26.70	0.50	0.5475
3.88	0.55	0.4451	10.98	0.55	0.5137	26.77	0.55	0.5681
3.85	0.60	0.4619	10.94	0.60	0.5331	26.78	0.60	0.5898
3.81	0.65	0.4810	10.86	0.65	0.5545	26.72	0.65	0.6131
3.74	0.70	0.5034	10.74	0.70	0.5790	26.57	0.70	0.6392
3.66	0.75	0.5309	10.57	0.75	0.6082	26.32	0.75	0.6693
3.54	0.80	0.5663	10.33	0.80	0.6443	25.93	0.80	0.7052
3.38	0.85	0.6145	9.99	0.85	0.6912	25.35	0.85	0.7496
3.15	0.90	0.6846	9.51	0.90	0.7553	24.53	0.90	0.8072
2.82	0.95	0.7962	8.83	0.95	0.8492	23.36	0.95	0.8857
2.36	1.00	1.0000	7.86	1.00	1.0000	21.69	1.00	1.0000
								390.85
<i>Q</i> <sub>0</sub> =0.397			<i>Q</i> <sub>0</sub> =0.364			<i>Q</i> <sub>1</sub> =0.252		
			<i>Q</i> <sub>0</sub> =0.328			<i>Q</i> <sub>0</sub> =0.254		
						$\sigma_1=0.46 \text{ kPa}$		
						$\sigma_0=0.48 \text{ kPa}$		

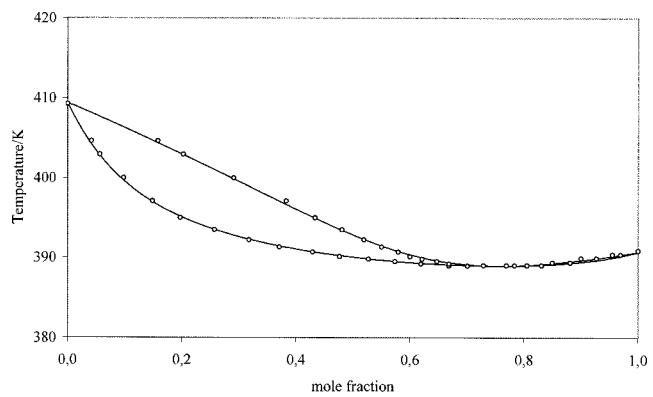
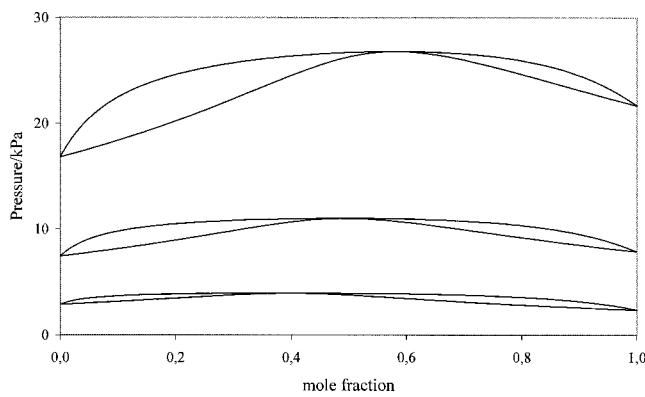


Table 3.14. 1-Pentanol–benzene

Components			References					
1-Pentanol, C <sub>5</sub> H <sub>12</sub> O [71-41-0]	Benzene, C <sub>6</sub> H <sub>6</sub> [71-43-2]		<sup>1</sup> J. M. Rhodes, T. A. Griffin, M. J. Lazzaroni, V. R. Bhethanabotla, and S. W. Campbell, Fluid Phase Equilib. <b>179</b> , 217 (2001).					
Reference vapor–liquid equilibrium data								
T/K=313.15, Ref. 1			T/K=333.15, predicted			T/K=353.15, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>
24.509	0.0000	0.0000	52.49	0.00	0.0000	101.59	0.00	0.0000
23.980	0.0305	0.0065	50.99	0.05	0.0124	98.73	0.05	0.0157
23.589	0.0606	0.0100	49.72	0.10	0.0192	96.15	0.10	0.0256
23.200	0.1010	0.0131	48.56	0.15	0.0240	93.72	0.15	0.0331
22.770	0.1503	0.0157	47.43	0.20	0.0280	91.31	0.20	0.0395
22.311	0.2007	0.0179	46.28	0.25	0.0316	88.87	0.25	0.0454
21.826	0.2508	0.0198	45.07	0.30	0.0351	86.32	0.30	0.0511
21.301	0.3016	0.0217	43.77	0.35	0.0386	83.61	0.35	0.0570
20.779	0.3508	0.0236	42.36	0.40	0.0424	80.68	0.40	0.0632
20.182	0.4010	0.0256	40.79	0.45	0.0465	77.50	0.45	0.0700
19.516	0.4507	0.0278	39.05	0.50	0.0512	74.00	0.50	0.0777
19.530	0.4512	0.0278	37.10	0.55	0.0566	70.14	0.55	0.0865
18.755	0.5012	0.0304	34.90	0.60	0.0632	65.87	0.60	0.0971
17.862	0.5514	0.0334	32.41	0.65	0.0714	61.12	0.65	0.1101
16.834	0.6019	0.0371	29.60	0.70	0.0820	55.85	0.70	0.1266
15.648	0.6520	0.0417	26.43	0.75	0.0963	49.99	0.75	0.1485
14.267	0.7023	0.0478	22.83	0.80	0.1168	43.47	0.80	0.1792
12.692	0.7521	0.0560	18.77	0.85	0.1489	36.22	0.85	0.2254
10.868	0.8023	0.0683	14.19	0.90	0.2064	28.17	0.90	0.3037
8.797	0.8518	0.0878	9.02	0.95	0.3402	19.25	0.95	0.4655
6.395	0.9025	0.1258	3.22	1.00	1.0000	9.38	1.00	1.0000
4.294	0.9424	0.1938						
2.520	0.9734	0.3401						
0.899	1.0000	1.0000						

$Q_1 = 0.310$	$\sigma_1 = 0.06 \text{ kPa}$		
$Q_0 = 0.308$	$\sigma_0 = 0.07 \text{ kPa}$	$Q_0 = 0.276$	$Q_0 = 0.243$

$Q_0 = 0.224$
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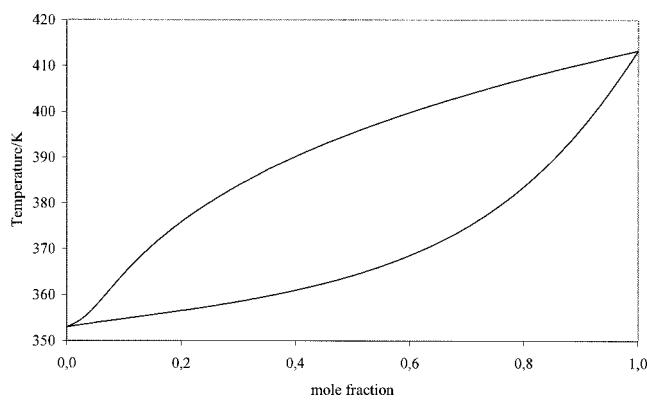
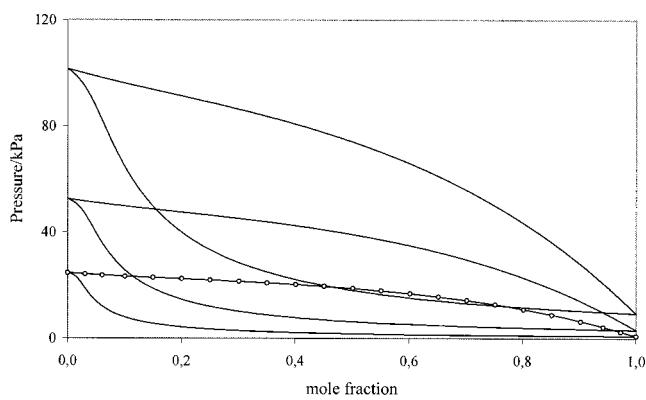


Table 3.15. 1-Hexanol–1,4-dimethylbenzene

Components				References							
1-Hexanol, C <sub>6</sub> H <sub>14</sub> O [111-27-3]				<sup>1</sup> A. Galska-Krajewska, Roczn. Chem. <b>41</b> , 609 (1967).							
1,4-Dimethylbenzene, C <sub>8</sub> H <sub>10</sub> [106-42-3]											
Reference vapor–liquid equilibrium data											
<i>T/K</i> =313.15, predicted		<i>T/K</i> =343.15, predicted		<i>T/K</i> =373.15, predicted		<i>P/kPa</i> =101.32, Ref. 1					
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>T/K</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>
2.64	0.00	0.0000	10.49	0.00	0.0000	32.03	0.00	0.0000	411.52	0.000	0.0000
2.68	0.05	0.0506	10.49	0.05	0.0419	32.20	0.05	0.0497	411.32	0.027	0.0327
2.67	0.10	0.0748	10.40	0.10	0.0670	32.09	0.10	0.0845	411.32	0.041	0.0480
2.64	0.15	0.0916	10.27	0.15	0.0855	31.83	0.15	0.1118	411.08	0.074	0.0803
2.61	0.20	0.1051	10.12	0.20	0.1008	31.48	0.20	0.1350	411.14	0.090	0.0946
2.58	0.25	0.1169	9.95	0.25	0.1144	31.06	0.25	0.1558	411.01	0.103	0.1056
2.54	0.30	0.1277	9.77	0.30	0.1271	30.58	0.30	0.1753	411.11	0.141	0.1354
2.50	0.35	0.1381	9.57	0.35	0.1393	30.03	0.35	0.1943	411.30	0.214	0.1860
2.45	0.40	0.1485	9.35	0.40	0.1516	29.43	0.40	0.2132	411.72	0.292	0.2348
2.39	0.45	0.1591	9.12	0.45	0.1643	28.76	0.45	0.2326	412.85	0.403	0.3020
2.33	0.50	0.1704	8.85	0.50	0.1779	28.02	0.50	0.2531	414.01	0.488	0.3555
2.26	0.55	0.1828	8.56	0.55	0.1927	27.19	0.55	0.2753	415.13	0.556	0.4020
2.19	0.60	0.1969	8.23	0.60	0.2097	26.25	0.60	0.2999	414.98	0.557	0.4024
2.09	0.65	0.2137	7.85	0.65	0.2295	25.19	0.65	0.3281	416.56	0.632	0.4601
1.98	0.70	0.2343	7.41	0.70	0.2537	23.98	0.70	0.3613	418.58	0.725	0.5446
1.85	0.75	0.2609	6.90	0.75	0.2844	22.59	0.75	0.4016	422.42	0.849	0.6969
1.69	0.80	0.2972	6.29	0.80	0.3253	20.99	0.80	0.4525	429.44	1.000	1.0000
1.50	0.85	0.3499	5.58	0.85	0.3835	19.14	0.85	0.5197			
1.26	0.90	0.4346	4.72	0.90	0.4738	16.97	0.90	0.6137			
0.97	0.95	0.5934	3.70	0.95	0.6340	14.44	0.95	0.7563			
0.60	1.00	1.0000	2.46	1.00	1.0000	11.45	1.00	1.0000			
<i>Q</i> <sub>0</sub> =0.329		<i>Q</i> <sub>0</sub> =0.288		<i>Q</i> <sub>0</sub> =0.241		<i>Q</i> <sub>1</sub> =0.164 $\sigma_1=0.43 \text{ kPa}$					
						<i>Q</i> <sub>0</sub> =0.173 $\sigma_0=0.85 \text{ kPa}$					

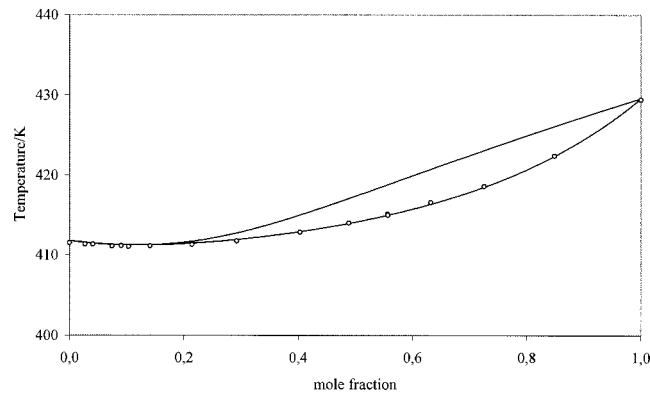
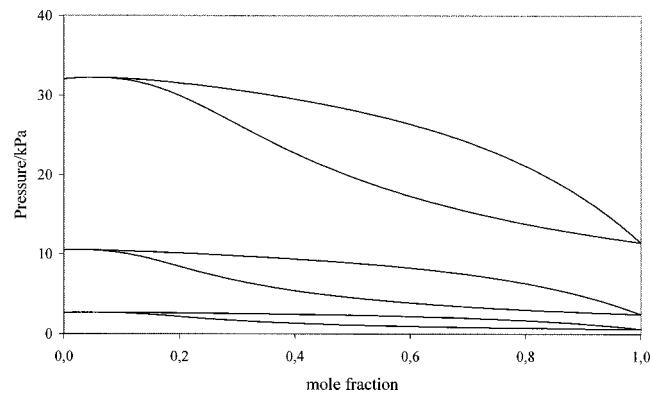


Table 3.16. 1-Hexanol–ethylbenzene

Components			References								
1-Hexanol, C <sub>6</sub> H <sub>14</sub> O [111-27-3]			<sup>1</sup> Z. Lisicki and A. Galska-Krajewska, Roczn. Chem. <b>40</b> , 873 (1966).								
Ethylbenzene, C <sub>8</sub> H <sub>10</sub> [100-41-4]											
Reference vapor–liquid equilibrium data											
T/K=313.15, predicted		T/K=343.15, predicted		T/K=373.15, predicted		P/kPa=101.32, Ref. 1					
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1,calc</sub>
2.86	0.00	0.0000	11.30	0.00	0.0000	34.26	0.00	0.0000	409.33	0.000	0.0000
2.88	0.05	0.0471	11.26	0.05	0.0389	34.30	0.05	0.0461	409.29	0.020	0.0237
2.87	0.10	0.0696	11.14	0.10	0.0622	34.09	0.10	0.0784	409.27	0.031	0.0356
2.84	0.15	0.0852	10.98	0.15	0.0795	33.74	0.15	0.1041	409.24	0.044	0.0489
2.80	0.20	0.0977	10.81	0.20	0.0939	33.31	0.20	0.1260	409.25	0.062	0.0660
2.76	0.25	0.1087	10.62	0.25	0.1066	32.81	0.25	0.1459	409.25	0.095	0.0944
2.72	0.30	0.1188	10.42	0.30	0.1185	32.24	0.30	0.1646	409.26	0.132	0.1226
2.67	0.35	0.1285	10.20	0.35	0.1301	31.62	0.35	0.1828	409.34	0.135	0.1248
2.62	0.40	0.1381	9.96	0.40	0.1418	30.93	0.40	0.2012	409.34	0.200	0.1683
2.56	0.45	0.1480	9.69	0.45	0.1539	30.18	0.45	0.2201	409.55	0.245	0.1958
2.49	0.50	0.1587	9.40	0.50	0.1668	29.34	0.50	0.2402	410.72	0.340	0.2515
2.42	0.55	0.1704	9.08	0.55	0.1811	28.41	0.55	0.2621	410.92	0.353	0.2591
2.33	0.60	0.1838	8.71	0.60	0.1975	27.36	0.60	0.2865	411.43	0.409	0.2915
2.23	0.65	0.1998	8.29	0.65	0.2167	26.19	0.65	0.3145	412.21	0.467	0.3265
2.11	0.70	0.2196	7.81	0.70	0.2403	24.86	0.70	0.3476	412.69	0.505	0.3504
1.96	0.75	0.2453	7.24	0.75	0.2704	23.34	0.75	0.3880	414.88	0.623	0.4347
1.79	0.80	0.2805	6.58	0.80	0.3107	21.60	0.80	0.4393	416.55	0.697	0.4989
1.57	0.85	0.3321	5.81	0.85	0.3683	19.60	0.85	0.5072	418.32	0.757	0.5611
1.31	0.90	0.4157	4.88	0.90	0.4583	17.28	0.90	0.6027	420.29	0.814	0.6317
0.99	0.95	0.5753	3.78	0.95	0.6202	14.59	0.95	0.7483	422.32	0.869	0.7138
0.60	1.00	1.0000	2.46	1.00	1.0000	11.45	1.00	1.0000	424.81	0.924	0.8151
									427.17	0.968	0.9145
									429.44	1.000	1.0000
$Q_0 = 0.329$			$Q_0 = 0.285$			$Q_0 = 0.235$			$Q_1 = 0.168$	$\sigma_1 = 0.49 \text{ kPa}$	
						$Q_0 = 0.164$			$Q_1 = 0.164$	$\sigma_0 = 0.58 \text{ kPa}$	

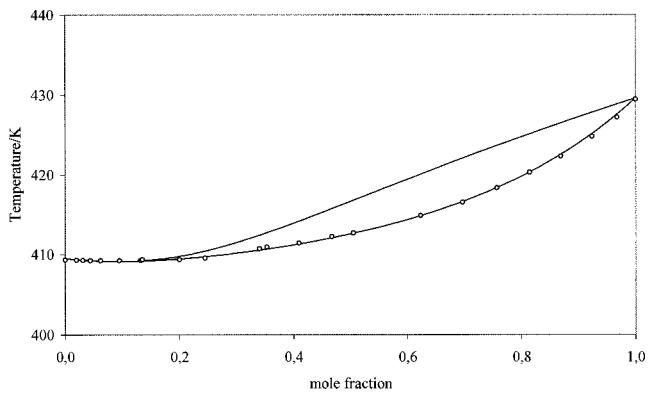
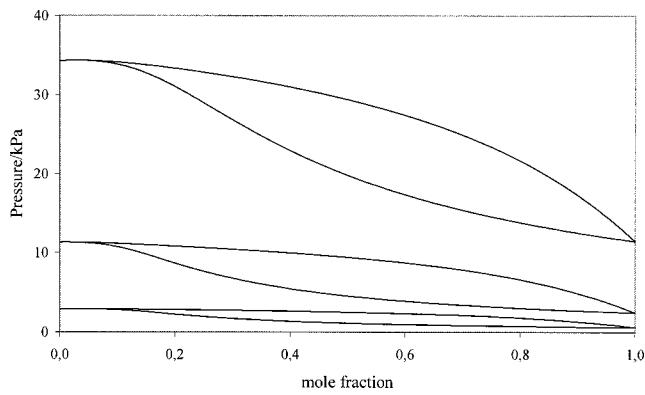


Table 3.17. 2-Propanol–benzene

Components			References		
2-propanol, C <sub>3</sub> H <sub>8</sub> O [67-63-0]			<sup>1</sup> I. Brown, W. Fock, and F. Smith, Aust. J. Chem. <b>9</b> , 364 (1956).		
Benzene, C <sub>6</sub> H <sub>6</sub> [71-43-2]			<sup>2</sup> I. Nagata, T. Ohta, and Y. Uchiyama, J. Chem. Eng. Data <b>18</b> , 54 (1973).		
			<sup>3</sup> V. T. Zharov, N. D. Malegina, and A. G. Morachevskii, Zh. Prikl. Khim. (Leningrad) <b>38</b> , 2132 (1965).		
Reference vapor–liquid equilibrium data					
<i>T/K</i> =318.15, Ref. 1			<i>T/K</i> =343.15, Ref. 2		
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
29.83	0.0000	0.0000	82.63	0.053	0.149
33.66	0.0472	0.1467	87.45	0.095	0.222
35.21	0.0980	0.2066	91.39	0.164	0.283
36.27	0.2047	0.2663	94.01	0.291	0.350
36.45	0.2960	0.2953	94.27	0.382	0.386
36.29	0.3862	0.3211	93.87	0.465	0.417
35.93	0.4753	0.3463	92.81	0.559	0.456
35.32	0.5504	0.3692	90.97	0.647	0.500
34.58	0.6198	0.3951	86.99	0.751	0.565
33.02	0.7096	0.4378	79.47	0.860	0.678
30.28	0.8073	0.5107			184.25
25.24	0.9120	0.6658			183.64
21.30	0.9655	0.8252			182.49
18.14	1.0000	1.0000			180.72
					178.22
					174.86
					170.45
					164.77
					157.54
					148.40
					136.94
<i>Q</i> <sub>1</sub> =0.380	$\sigma_1=0.10 \text{ kPa}$	<i>Q</i> <sub>1</sub> =0.322	$\sigma_1=0.49 \text{ kPa}$	$Q_0=0.285$	<i>Q</i> <sub>1</sub> =0.321
<i>Q</i> <sub>0</sub> =0.378	$\sigma_0=0.12 \text{ kPa}$	<i>Q</i> <sub>0</sub> =0.327	$\sigma_0=0.64 \text{ kPa}$		$Q_0=0.323$
					$\sigma_1=0.18 \text{ kPa}$
					$\sigma_0=0.24 \text{ kPa}$

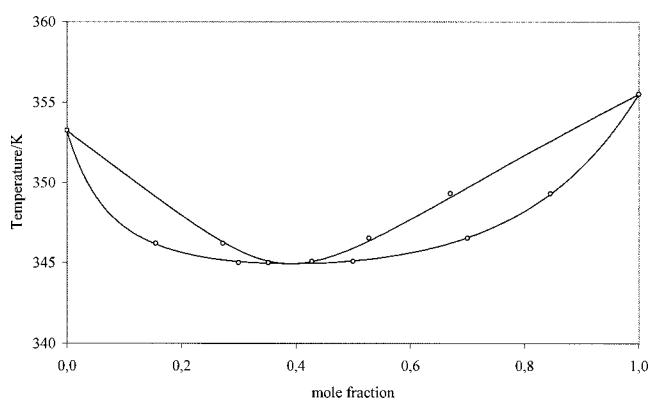
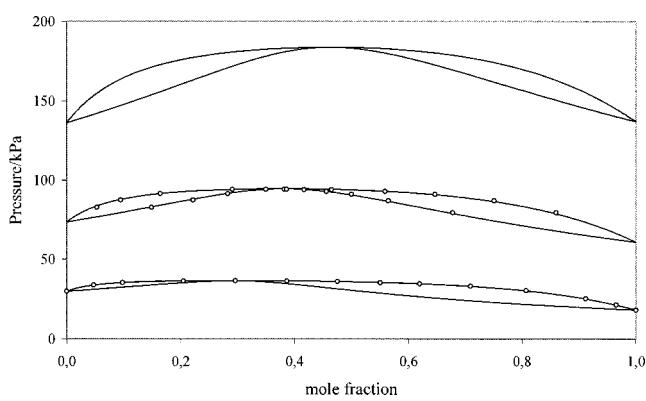


Table 3.18. 2-Propanol–ethylbenzene

Components			References								
2-propanol, C <sub>3</sub> H <sub>8</sub> O [67-63-0]			<sup>1</sup> C. De Alfonso, M. Pintado, and A. F. Saenz Dela Torre, An. Quim., Ser. A <b>79</b> , 254 (1983).								
Ethylbenzene, C <sub>8</sub> H <sub>10</sub> [100-41-4]											
Reference vapor–liquid equilibrium data											
T/K=313.15, predicted		T/K=343.15, predicted		T/K=373.15, predicted		P/kPa=101.33, Ref. 1					
P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	T/K	x <sub>1</sub>	y <sub>1</sub>
2.86	0.00	0.0000	11.27	0.00	0.0000	34.15	0.00	0.0000	409.45	0.0000	0.0000
7.36	0.05	0.6260	25.04	0.05	0.5662	65.76	0.05	0.4974	396.95	0.0280	0.3120
9.31	0.10	0.7121	32.93	0.10	0.6804	87.85	0.10	0.6357	393.25	0.0370	0.3900
10.41	0.15	0.7481	38.06	0.15	0.7310	104.15	0.15	0.7021	389.65	0.0490	0.4600
11.13	0.20	0.7688	41.68	0.20	0.7606	116.72	0.20	0.7421	386.55	0.0620	0.5110
11.64	0.25	0.7829	44.39	0.25	0.7806	126.77	0.25	0.7695	383.85	0.0720	0.5500
12.03	0.30	0.7935	46.53	0.30	0.7956	135.05	0.30	0.7900	380.15	0.0870	0.6070
12.34	0.35	0.8021	48.28	0.35	0.8077	142.04	0.35	0.8064	378.35	0.1050	0.6390
12.60	0.40	0.8096	49.75	0.40	0.8179	148.10	0.40	0.8201	374.10	0.1340	0.6980
12.82	0.45	0.8163	51.03	0.45	0.8271	153.46	0.45	0.8322	372.20	0.1480	0.7150
13.01	0.50	0.8228	52.17	0.50	0.8356	158.30	0.50	0.8433	370.45	0.1690	0.7340
13.19	0.55	0.8292	53.21	0.55	0.8439	162.76	0.55	0.8538	369.25	0.1920	0.7515
13.36	0.60	0.8360	54.19	0.60	0.8523	166.94	0.60	0.8641	366.25	0.2540	0.7860
13.52	0.65	0.8434	55.12	0.65	0.8612	170.93	0.65	0.8746	364.90	0.2920	0.7970
13.67	0.70	0.8519	56.02	0.70	0.8709	174.81	0.70	0.8856	364.70	0.2990	0.7995
13.82	0.75	0.8622	56.91	0.75	0.8820	178.62	0.75	0.8975	364.05	0.3210	0.8065
13.97	0.80	0.8751	57.79	0.80	0.8952	182.40	0.80	0.9109	363.95	0.3240	0.8085
14.10	0.85	0.8921	58.64	0.85	0.9115	186.18	0.85	0.9266	363.10	0.3620	0.8165
14.21	0.90	0.9154	59.44	0.90	0.9324	189.91	0.90	0.9455	362.20	0.4100	0.8270
14.24	0.95	0.9490	60.10	0.95	0.9605	193.52	0.95	0.9691	360.80	0.4880	0.8450
14.15	1.00	1.0000	60.48	1.00	1.0000	196.79	1.00	1.0000	360.20	0.5270	0.8495
									359.15	0.6100	0.8640
									358.60	0.6550	0.8740
									358.25	0.6850	0.8790
									357.65	0.7455	0.8945
									357.30	0.7875	0.9045
									356.90	0.8200	0.9150
									356.75	0.8465	0.9215
									356.45	0.8740	0.9320
									356.10	0.9040	0.9445
									355.95	0.9280	0.9560
									355.75	0.9530	0.9680
									355.65	0.9740	0.9820
									355.55	0.9840	0.9895
									355.55	1.0000	1.0000

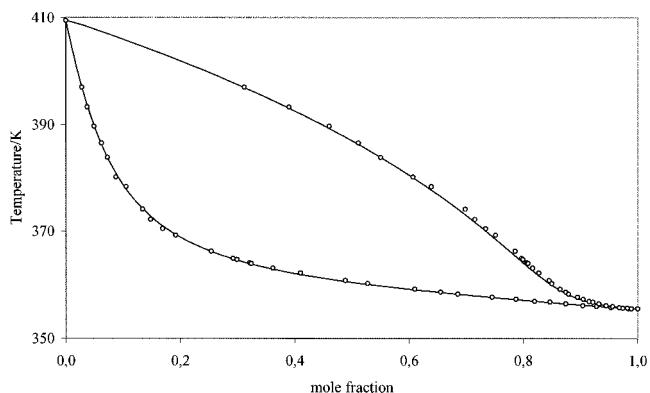
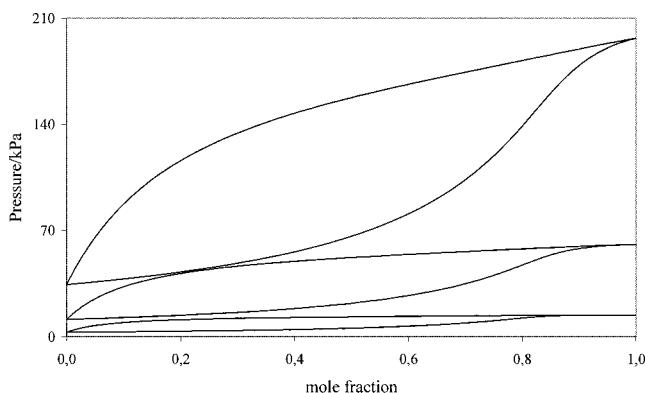


Table 3.19. 2-Methyl-1-propanol–benzene

Components			References		
2-Methyl-1-propanol, C <sub>4</sub> H <sub>10</sub> O [78-83-1]			<sup>1</sup> B. B. Allen, S. P. Lingo, and W. A. Felsing, J. Phys. Chem. <b>43</b> , 425 (1939).		
Benzene, C <sub>6</sub> H <sub>6</sub> [71-43-2]			<sup>2</sup> I. Brown, W. Fock, and F. Smith, J. Chem. Thermodyn. <b>1</b> , 273 (1969).		
			<sup>3</sup> H. Ruiz Echevarria, Collect. Czech. Chem. Commun. <b>38</b> , 1295 (1973).		
Reference vapor–liquid equilibrium data					
<i>T/K</i> =298.15, Ref. 1			<i>T/K</i> =318.15, Ref. 2		
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
12.59	0.000	0.0000	29.77	0.0000	0.0000
12.43	0.202	0.0708	30.01	0.0464	0.0451
11.91	0.343	0.0844	29.85	0.1007	0.0689
11.16	0.498	0.1005	29.12	0.2162	0.0944
10.04	0.640	0.1237	28.50	0.2964	0.1072
7.57	0.805	0.1855	27.10	0.4333	0.1275
1.68	1.000	1.0000	26.08	0.5096	0.1405
			24.74	0.5879	0.1568
			22.44	0.7004	0.1910
			18.55	0.7989	0.2445
			14.79	0.8716	0.3269
			5.38	1.0000	1.0000
<i>T/K</i> =353.15, Ref. 3			<i>P/kPa</i> =101.32, predicted		
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>T/K</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
12.59	0.000	0.0000	353.22	0.00	0.0000
12.43	0.202	0.0708	352.59	0.05	0.0601
11.91	0.343	0.0844	352.51	0.10	0.0946
11.16	0.498	0.1005	352.66	0.15	0.1191
10.04	0.640	0.1237	352.92	0.20	0.1389
7.57	0.805	0.1855	353.27	0.25	0.1564
1.68	1.000	1.0000	353.71	0.30	0.1731
			354.23	0.35	0.1899
			354.84	0.40	0.2074
			355.57	0.45	0.2262
			356.43	0.50	0.2473
			357.45	0.55	0.2712
			358.66	0.60	0.2993
			360.10	0.65	0.3328
			361.81	0.70	0.3735
			363.85	0.75	0.4242
			366.27	0.80	0.4881
			369.14	0.85	0.5702
			372.51	0.90	0.6768
			376.43	0.95	0.8165
			380.91	1.00	1.0000
<i>Q</i> <sub>1</sub> =0.378	<i>σ</i> <sub>1</sub> =0.04 kPa	<i>Q</i> <sub>1</sub> =0.351	<i>σ</i> <sub>1</sub> =0.19 kPa	<i>Q</i> <sub>1</sub> =0.274	<i>σ</i> <sub>1</sub> =0.55 kPa
<i>Q</i> <sub>0</sub> =0.381	<i>σ</i> <sub>0</sub> =0.05 kPa	<i>Q</i> <sub>0</sub> =0.344	<i>σ</i> <sub>0</sub> =0.25 kPa	<i>Q</i> <sub>0</sub> =0.272	<i>σ</i> <sub>0</sub> =0.56 kPa
					<i>Q</i> <sub>0</sub> =0.265

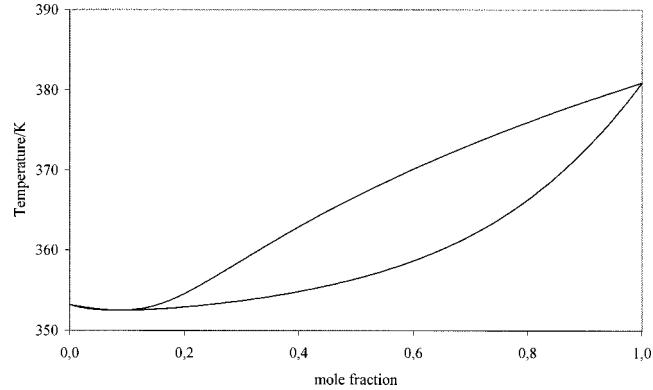
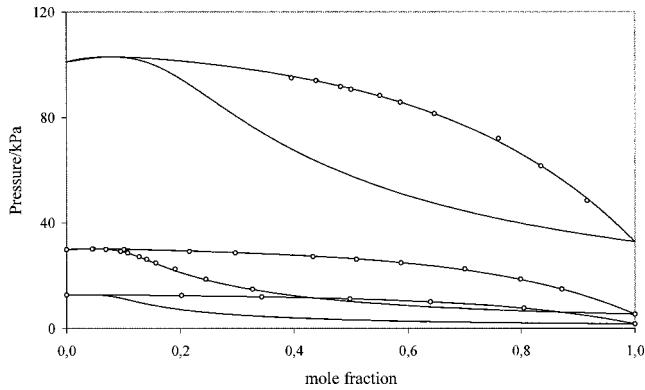


Table 3.20. 2-Methyl-1-propanol–toluene

Components			References		
2-Methyl-1-propanol, C <sub>4</sub> H <sub>10</sub> O [78-83-1]			<sup>1</sup> P. Oracz, Int. DATA Ser., Sel. Data Mixtures, Ser. A <b>17</b> , 232 (1989).		
Toluene, C <sub>7</sub> H <sub>8</sub> [108-88-3]			<sup>2</sup> J. Lnenickova and I. Wichterle, Collect. Czech. Chem. Commun. <b>42</b> , 1907 (1977).		
			<sup>3</sup> V. Martinez-Soria, M. P. Pena, and J. B. Monton, J. Chem. Eng. Data <b>44</b> , 608 (1999).		
Reference vapor–liquid equilibrium data					
<i>T/K</i> =313.15, Ref. 1			<i>T/K</i> =343.4, Ref. 2		
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
7.894	0.00000	0.0000	27.42	0.000	0.000
8.570	0.03433	0.1086	27.73	0.003	0.009
8.702	0.04565	0.1277	29.25	0.028	0.081
8.834	0.05497	0.1405	32.29	0.104	0.216
9.129	0.10210	0.1840	33.62	0.198	0.282
9.229	0.15220	0.2116	34.11	0.289	0.328
9.277	0.19940	0.2304	34.11	0.407	0.375
9.265	0.25230	0.2473	33.84	0.489	0.407
9.129	0.39930	0.2857	32.97	0.606	0.459
8.981	0.48050	0.3064	32.21	0.683	0.498
8.601	0.60180	0.3429	30.37	0.783	0.573
8.189	0.70310	0.3863	29.32	0.824	0.617
7.933	0.74480	0.4108	28.51	0.854	0.657
7.582	0.79480	0.4488	26.14	0.915	0.749
6.906	0.85680	0.5175	24.81	0.943	0.816
6.243	0.90080	0.5922	23.26	0.972	0.898
5.289	0.95020	0.7285	21.44	1.000	1.000
4.029	1.00000	1.0000			
<i>Q</i> <sub>1</sub> =0.387 $\sigma_1=0.04 \text{ kPa}$			<i>Q</i> <sub>1</sub> =0.316 $\sigma_1=0.13 \text{ kPa}$		
<i>Q</i> <sub>0</sub> =0.381 $\sigma_0=0.06 \text{ kPa}$			<i>Q</i> <sub>0</sub> =0.322 $\sigma_0=0.19 \text{ kPa}$		
			<i>Q</i> <sub>0</sub> =0.258		
			<i>Q</i> <sub>1</sub> =0.260 $\sigma_1=0.24 \text{ kPa}$		
			<i>Q</i> <sub>0</sub> =0.256 $\sigma_0=0.46 \text{ kPa}$		

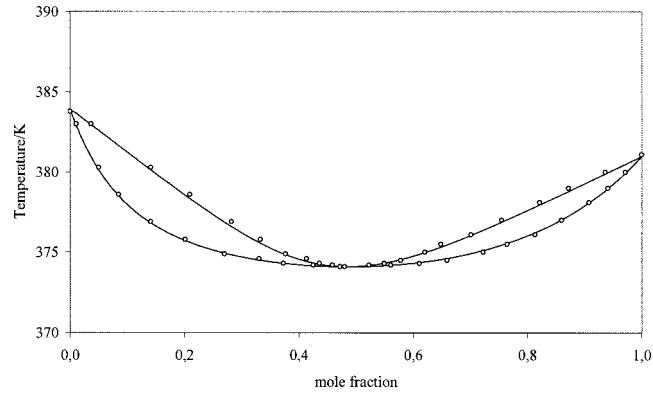
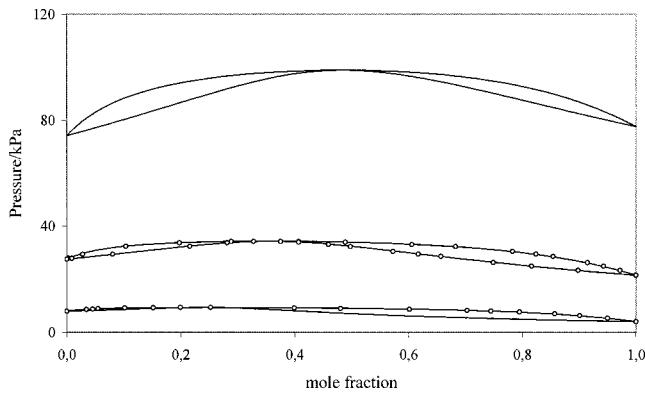


Table 3.21. 2-Methyl-1-propanol–1,4-dimethylbenzene

Components			References		
2-Methyl-1-propanol, C <sub>4</sub> H <sub>10</sub> O [78-83-1]			<sup>1</sup> P. Oracz, Int. DATA Ser., Sel. Data Mixtures, Ser. A <b>17</b> , 238 (1989).		
Reference vapor–liquid equilibrium data					
<i>T</i> /K = 313.15, Ref. 1		<i>T</i> /K = 343.15, predicted		<i>T</i> /K = 373.15, predicted	
<i>P</i> /kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P</i> /kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
2.652	0.00000	0.0000	10.52	0.00	0.0000
3.485	0.03560	0.2741	14.80	0.05	0.3167
3.841	0.05826	0.3395	17.04	0.10	0.4256
4.044	0.07700	0.3747	18.46	0.15	0.4848
4.202	0.10250	0.4087	19.46	0.20	0.5243
4.474	0.15430	0.4540	20.22	0.25	0.5541
4.688	0.23160	0.4962	20.82	0.30	0.5784
4.733	0.24650	0.5027	21.30	0.35	0.5993
4.818	0.30380	0.5245	21.71	0.40	0.6183
4.932	0.40030	0.5550	22.04	0.45	0.6360
4.984	0.49700	0.5826	22.33	0.50	0.6531
4.997	0.58970	0.6099	22.57	0.55	0.6703
4.981	0.69890	0.6490	22.76	0.60	0.6881
4.950	0.74330	0.6694	22.91	0.65	0.7070
4.893	0.78710	0.6938	23.01	0.70	0.7279
4.782	0.84790	0.7387	23.05	0.75	0.7518
4.593	0.90760	0.8040	23.01	0.80	0.7800
4.398	0.94890	0.8708	22.87	0.85	0.8145
4.029	1.00000	1.0000	22.58	0.90	0.8585
			22.06	0.95	0.9173
			21.21	1.00	1.0000

<i>Q</i> <sub>1</sub> =0.406	$\sigma_1=0.03 \text{ kPa}$	<i>Q</i> <sub>0</sub> =0.407	$\sigma_0=0.02 \text{ kPa}$	<i>Q</i> <sub>0</sub> =0.350	<i>Q</i> <sub>0</sub> =0.287	<i>Q</i> <sub>0</sub> =0.266
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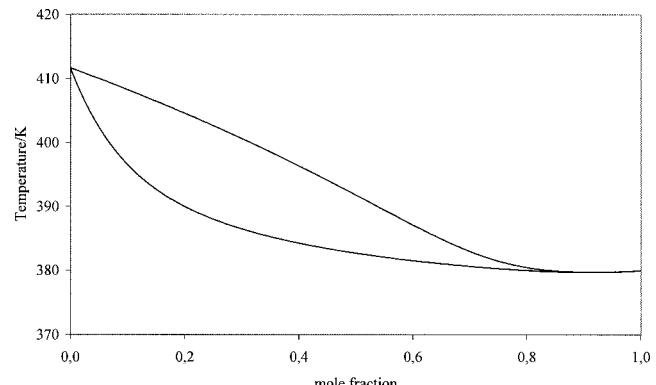
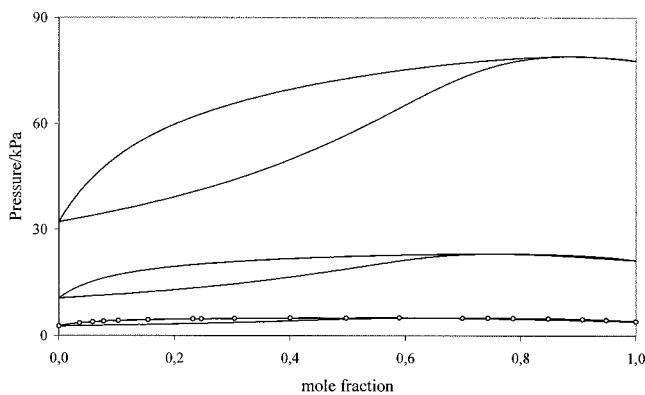


Table 3.22. 2-Methyl-1-propanol–ethylbenzene

Components			References		
2-Methyl-1-propanol, C <sub>4</sub> H <sub>10</sub> O [78-83-1]			<sup>1</sup> P. Oracz, Thesis, Warsaw University, Warsaw, 1976.		
Ethylbenzene, C <sub>8</sub> H <sub>10</sub> [100-41-4]					
Reference vapor–liquid equilibrium data					
<i>T/K</i> =313.15, Ref. 1		<i>T/K</i> =343.15, predicted		<i>T/K</i> =373.15, predicted	
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
2.87	0.0000	0.0000	11.32	0.00	0.0000
4.41	0.1026	0.3895	15.54	0.05	0.3006
4.46	0.1060	0.3931	17.75	0.10	0.4071
4.78	0.1923	0.4567	19.14	0.15	0.4656
4.91	0.2516	0.4842	20.12	0.20	0.5051
4.96	0.2825	0.4962	20.85	0.25	0.5350
5.08	0.4017	0.5348	21.42	0.30	0.5595
5.16	0.4828	0.5582	21.89	0.35	0.5807
5.16	0.6005	0.5937	22.27	0.40	0.6000
5.12	0.6941	0.6286	22.59	0.45	0.6181
5.08	0.7413	0.6508	22.85	0.50	0.6357
5.00	0.7875	0.6777	23.07	0.55	0.6535
4.90	0.8353	0.7133	23.24	0.60	0.6719
4.69	0.8965	0.7780	23.36	0.65	0.6917
4.48	0.9401	0.8463	23.42	0.70	0.7136
4.03	1.0000	1.0000	23.42	0.75	0.7386
			23.34	0.80	0.7683
			23.14	0.85	0.8047
			22.77	0.90	0.8511
			22.17	0.95	0.9130
			21.22	1.00	1.0000
<i>Q</i> <sub>1</sub> =0.404		<i>σ</i> <sub>1</sub> =0.02 kPa	<i>Q</i> <sub>0</sub> =0.347		<i>Q</i> <sub>0</sub> =0.281
<i>Q</i> <sub>0</sub> =0.407		<i>σ</i> <sub>0</sub> =0.02 kPa			<i>Q</i> <sub>0</sub> =0.260

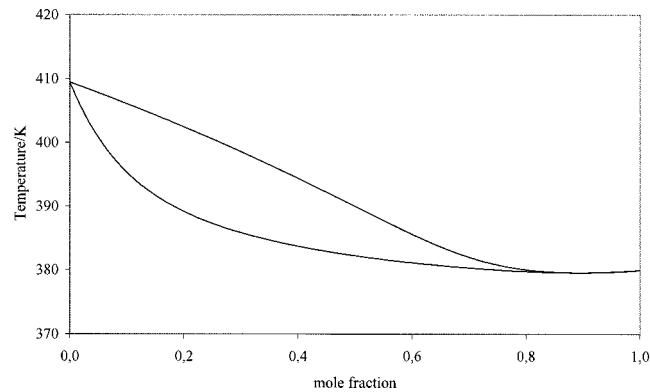
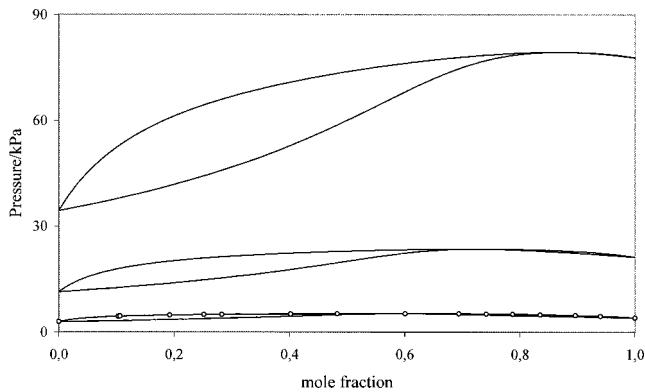


Table 3.23. 2-Butanol–benzene

Components			References								
2-Butanol, C <sub>4</sub> H <sub>10</sub> O [78-92-2]			<sup>1</sup> B. B. Allen, S. P. Lingo, and W. A. Felsing, J. Phys. Chem. <b>43</b> , 425 (1939).								
Benzene, C <sub>6</sub> H <sub>6</sub> [71-43-2]			<sup>2</sup> I. Brown, W. Fock, and F. Smith, J. Chem. Thermodyn. <b>1</b> , 273 (1969).								
Reference vapor–liquid equilibrium data											
<i>T/K</i> =298.15, Ref. 1		<i>T/K</i> =318.15, Ref. 2		<i>T/K</i> =338.15, predicted							
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>T/K</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
12.59	0.000	0.0000	29.77	0.0000	0.0000	62.04	0.00	0.0000	353.25	0.00	0.0000
12.85	0.095	0.0735	30.49	0.0607	0.0687	63.57	0.05	0.0650	352.55	0.05	0.0639
12.68	0.197	0.0965	30.47	0.1018	0.0915	63.91	0.10	0.1018	352.34	0.10	0.1051
12.13	0.353	0.1193	29.94	0.2093	0.1275	63.77	0.15	0.1275	352.37	0.15	0.1362
11.39	0.500	0.1421	29.25	0.3052	0.1507	63.36	0.20	0.1480	352.55	0.20	0.1623
10.25	0.646	0.1764	28.41	0.3933	0.1714	62.78	0.25	0.1657	352.82	0.25	0.1858
8.09	0.797	0.2508	27.03	0.5081	0.2003	62.04	0.30	0.1821	353.19	0.30	0.2083
2.45	1.000	1.0000	25.39	0.6046	0.2299	61.17	0.35	0.1981	353.64	0.35	0.2308
			23.09	0.7030	0.2738	60.13	0.40	0.2143	354.19	0.40	0.2541
			19.90	0.7997	0.3436	58.93	0.45	0.2313	354.84	0.45	0.2789
			15.47	0.8943	0.4791	57.54	0.50	0.2496	355.60	0.50	0.3059
			8.12	1.0000	1.0000	55.92	0.55	0.2699	356.48	0.55	0.3359
						54.04	0.60	0.2930	357.52	0.60	0.3699
						51.86	0.65	0.3199	358.71	0.65	0.4091
						49.33	0.70	0.3523	360.10	0.70	0.4548
						46.39	0.75	0.3922	361.69	0.75	0.5089
						42.98	0.80	0.4432	363.52	0.80	0.5736
						39.02	0.85	0.5112	365.61	0.85	0.6515
						34.43	0.90	0.6068	367.96	0.90	0.7460
						29.11	0.95	0.7521	370.59	0.95	0.8607
						22.95	1.00	1.0000	373.50	1.00	1.0000
<i>Q</i> <sub>1</sub> =0.360		<i>σ</i> <sub>1</sub> =0.05 kPa	<i>Q</i> <sub>1</sub> =0.321		<i>σ</i> <sub>1</sub> =0.14 kPa						
<i>Q</i> <sub>0</sub> =0.360		<i>σ</i> <sub>0</sub> =0.04 kPa	<i>Q</i> <sub>0</sub> =0.320		<i>σ</i> <sub>0</sub> =0.14 kPa						
								<i>Q</i> <sub>0</sub> =0.277			<i>Q</i> <sub>0</sub> =0.238

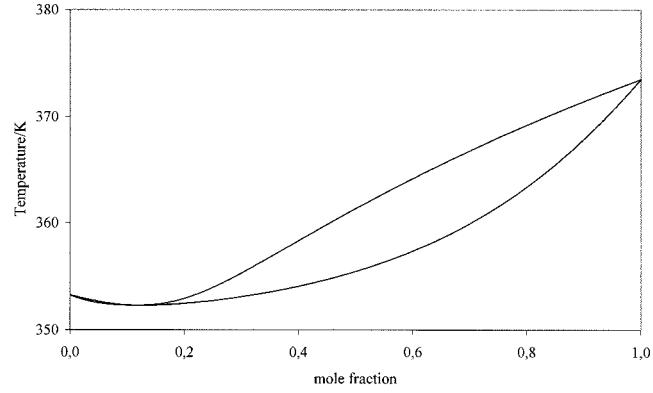
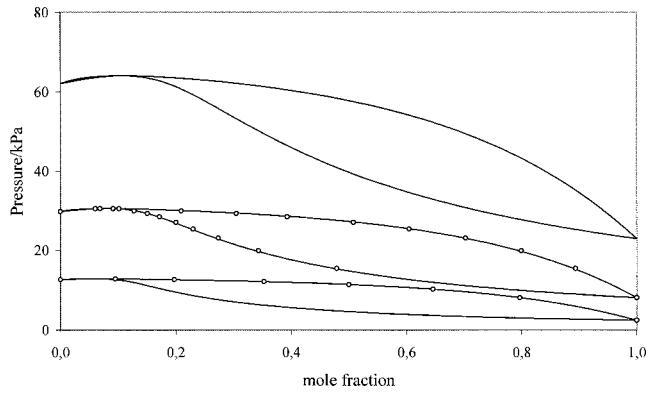


Table 3.24. 2-Butanol–toluene

Components			References								
2-Butanol, C <sub>4</sub> H <sub>10</sub> O [78-92-2]			<sup>1</sup> J. Lnenickova and I. Wichterle, Collect. Czech. Chem. Commun. <b>42</b> , 1907 (1977).								
Toluene, C <sub>7</sub> H <sub>8</sub> [108-88-3]											
Reference vapor–liquid equilibrium data											
<i>T/K</i> =313.15, predicted		<i>T/K</i> =333.31, Ref. 1		<i>T/K</i> =353.44, Ref. 1							
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>T/K</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
7.89	0.00	0.0000	18.64	0.000	0.000	39.22	0.000	0.000	383.90	0.00	0.0000
9.11	0.05	0.1680	18.94	0.004	0.017	39.70	0.005	0.017	379.83	0.05	0.1489
9.61	0.10	0.2340	21.07	0.041	0.141	44.04	0.041	0.130	377.16	0.10	0.2448
9.88	0.15	0.2731	22.71	0.083	0.226	46.14	0.068	0.197	375.32	0.15	0.3125
10.03	0.20	0.3013	23.74	0.125	0.278	51.96	0.166	0.332	373.99	0.20	0.3644
10.13	0.25	0.3240	24.34	0.166	0.313	54.62	0.268	0.406	372.98	0.25	0.4067
10.18	0.30	0.3437	25.14	0.270	0.372	55.45	0.322	0.439	372.21	0.30	0.4431
10.20	0.35	0.3617	25.37	0.332	0.400	56.64	0.427	0.493	371.60	0.35	0.4759
10.20	0.40	0.3790	25.58	0.432	0.446	57.00	0.541	0.547	371.12	0.40	0.5063
10.17	0.45	0.3962	25.50	0.543	0.497	55.91	0.731	0.665	370.75	0.45	0.5355
10.12	0.50	0.4139	24.31	0.742	0.611	54.93	0.796	0.714	370.46	0.50	0.5643
10.04	0.55	0.4327	23.59	0.798	0.658	53.09	0.866	0.785	370.25	0.55	0.5932
9.93	0.60	0.4535	22.27	0.873	0.738	49.72	0.946	0.926	370.11	0.60	0.6231
9.78	0.65	0.4771	19.76	0.966	0.911	47.27	1.000	1.000	370.05	0.65	0.6545
9.58	0.70	0.5048	18.49	1.000	1.000				370.07	0.70	0.6882
9.32	0.75	0.5383							370.18	0.75	0.7249
8.98	0.80	0.5804							370.38	0.80	0.7657
8.53	0.85	0.6355							370.70	0.85	0.8119
7.96	0.90	0.7112							371.14	0.90	0.8649
7.20	0.95	0.8220							371.74	0.95	0.9267
6.21	1.00	1.0000							372.53	1.00	1.0000
$Q_1 = 0.316$		$\sigma_1 = 0.08 \text{ kPa}$	$Q_1 = 0.272$		$\sigma_1 = 0.26 \text{ kPa}$	$Q_1 = 0.272$		$\sigma_1 = 0.26 \text{ kPa}$	$Q_1 = 0.273$		$\sigma_1 = 0.26 \text{ kPa}$
$Q_0 = 0.358$		$Q_0 = 0.317$	$\sigma_0 = 0.07 \text{ kPa}$		$\sigma_0 = 0.273$	$Q_0 = 0.273$		$\sigma_0 = 0.26 \text{ kPa}$	$Q_0 = 0.235$		

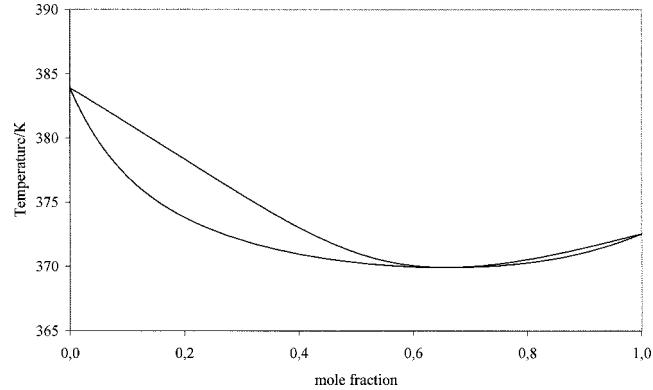
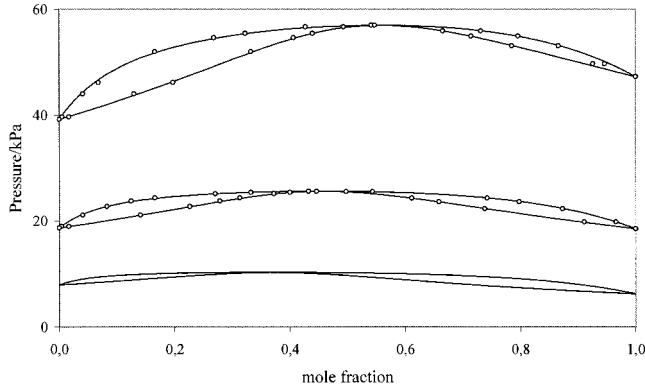


Table 3.25. 2-Methyl-2-propanol–benzene

Components			References					
2-Methyl-2-propanol, C <sub>4</sub> H <sub>10</sub> O [75-85-4]			<sup>1</sup> B. B. Allen, S. P. Lingo, and W. A. Felsing, J. Phys. Chem. <b>43</b> , 425 (1939).					
Benzene, C <sub>6</sub> H <sub>6</sub> [71-43-2]			<sup>2</sup> I. Brown, W. Fock, and F. Smith, J. Chem. Thermodyn. <b>1</b> , 273 (1969).					
<sup>3</sup> S. Govindaswamy, A. Andiappan, and S. M. Lakshmanan, J. Chem. Eng. Data <b>22</b> , 264 (1977).								
Reference vapor–liquid equilibrium data								
<i>T/K</i> =298.15, Ref. 1			<i>T/K</i> =318.15, Ref. 2					
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>			
12.59	0.000	0.0000	29.77	0.0000	0.0000			
13.96	0.100	0.1531	32.35	0.0475	0.1154			
14.08	0.198	0.1967	33.53	0.1012	0.1751			
13.91	0.351	0.2384	34.20	0.1788	0.2251			
13.36	0.499	0.2773	34.32	0.2924	0.2749			
12.37	0.652	0.3344	34.05	0.4027	0.3170			
10.73	0.802	0.4407	33.23	0.5136	0.3609			
5.61	1.000	1.0000	32.03	0.6147	0.4082			
			30.57	0.6993	0.4582			
			28.13	0.7945	0.5388			
			23.84	0.9060	0.6975			
			21.35	0.9514	0.8126			
			18.12	1.0000	1.0000			
<i>T/K</i> =338.15, predicted			<i>P/kPa</i> =101.32, Ref. 3					
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>	<i>T/K</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>			
62.04	0.00	0.0000	353.25	0.0000	0.0000			
67.54	0.05	0.1198	352.05	0.0200	0.0585			
70.46	0.10	0.1864	349.05	0.1000	0.1961			
72.17	0.15	0.2316	347.40	0.1960	0.2810			
73.21	0.20	0.2663	346.95	0.2575	0.3196			
73.82	0.25	0.2952	346.65	0.3320	0.3595			
74.12	0.30	0.3209	346.65	0.4125	0.4000			
74.19	0.35	0.3449	346.75	0.4650	0.4265			
74.05	0.40	0.3683	347.10	0.5500	0.4725			
73.71	0.45	0.3918	347.85	0.6625	0.5445			
73.17	0.50	0.4162	348.50	0.7160	0.5865			
72.41	0.55	0.4422	349.50	0.7850	0.6513			
71.41	0.60	0.4705	350.10	0.8200	0.6901			
70.14	0.65	0.5021	351.85	0.8990	0.7985			
68.55	0.70	0.5381	352.60	0.9230	0.8389			
66.59	0.75	0.5799	353.15	0.9400	0.8700			
64.21	0.80	0.6298	354.00	0.9600	0.9097			
61.33	0.85	0.6906	355.45	1.0000	1.0000			
57.86	0.90	0.7668						
53.72	0.95	0.8658						
8.78	1.00	1.0000						
<i>Q</i> <sub>1</sub> =0.356 <i>σ</i> <sub>1</sub> =0.06 kPa <i>Q</i> <sub>1</sub> =0.314 <i>σ</i> <sub>1</sub> =0.10 kPa <i>Q</i> <sub>0</sub> =0.268 <i>Q</i> <sub>1</sub> =0.255 <i>σ</i> <sub>1</sub> =0.44 kPa								
<i>Q</i> <sub>0</sub> =0.349 <i>σ</i> <sub>0</sub> =0.11 kPa <i>Q</i> <sub>0</sub> =0.310 <i>σ</i> <sub>0</sub> =0.15 kPa <i>Q</i> <sub>0</sub> =0.249 <i>Q</i> <sub>0</sub> =0.249 <i>σ</i> <sub>0</sub> =0.70 kPa								

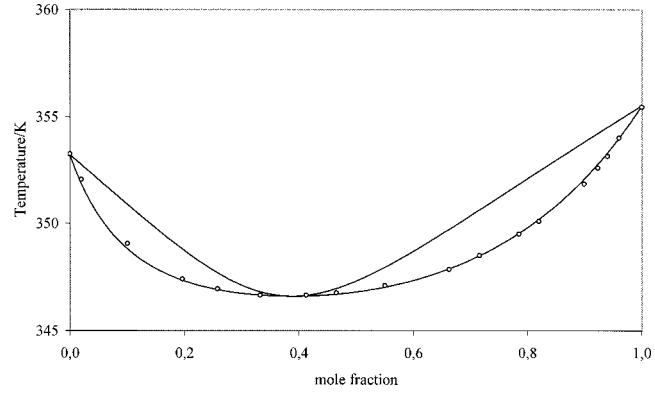
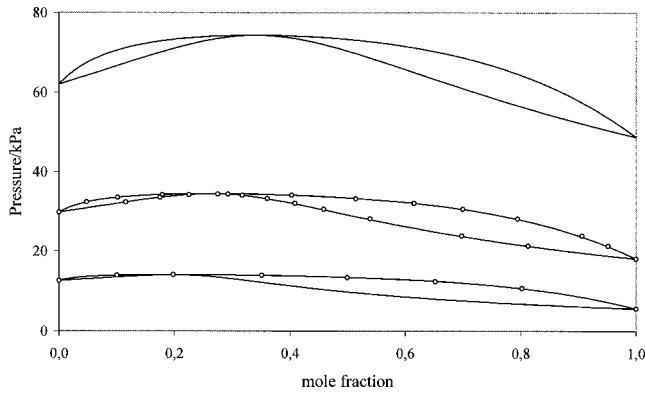


Table 3.26. 2-Methyl-2-propanol–toluene

Components			References		
2-Methyl-2-propanol, C <sub>4</sub> H <sub>10</sub> O [75-85-4]			<sup>1</sup> P. Oracz, Int. DATA Ser., Sel. Data Mixtures, Ser. A <b>17</b> , 244 (1989).		
Toluene, C <sub>7</sub> H <sub>8</sub> [108-88-3]			<sup>2</sup> J. Lnenickova and I. Wichterle, Collect. Czech. Chem. Commun. <b>42</b> , 1907 (1977).		
Reference vapor–liquid equilibrium data					
<i>T/K</i> =313.15, Ref. 1		<i>T/K</i> =333.15, predicted		<i>T/K</i> =353.44, Ref. 2	
<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P/kPa</i>	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
7.893	0.00000	0.0000	18.54	0.00	0.0000
10.111	0.03411	0.2374	24.95	0.05	0.2868
12.183	0.09700	0.3889	28.71	0.10	0.4016
13.072	0.14980	0.4485	31.23	0.15	0.4672
13.506	0.19080	0.4802	33.07	0.20	0.5119
14.186	0.28440	0.5315	34.49	0.25	0.5458
14.755	0.40130	0.5785	35.63	0.30	0.5735
15.073	0.48960	0.6101	36.57	0.35	0.5974
15.293	0.58310	0.6448	37.37	0.40	0.6190
15.381	0.69160	0.6921	38.05	0.45	0.6393
15.337	0.75540	0.7271	38.63	0.50	0.6590
15.300	0.78550	0.7463	39.14	0.55	0.6788
15.147	0.84200	0.7893	39.57	0.60	0.6992
14.944	0.88770	0.8329	39.93	0.65	0.7209
14.539	0.94190	0.8998	40.22	0.70	0.7447
13.787	1.00000	1.0000	40.41	0.75	0.7712
			40.49	0.80	0.8016
			40.42	0.85	0.8372
			40.17	0.90	0.8800
			39.67	0.95	0.9329
			38.83	1.00	1.0000
<i>Q</i> <sub>1</sub> =0.345 <i>σ</i> <sub>1</sub> =0.07 kPa		<i>Q</i> <sub>1</sub> =0.265 <i>σ</i> <sub>1</sub> =0.32 kPa		<i>Q</i> <sub>0</sub> =0.347 <i>σ</i> <sub>0</sub> =0.07 kPa	
		<i>Q</i> <sub>0</sub> =0.308		<i>Q</i> <sub>0</sub> =0.265 <i>σ</i> <sub>0</sub> =0.31 kPa	
				<i>Q</i> <sub>0</sub> =0.255	

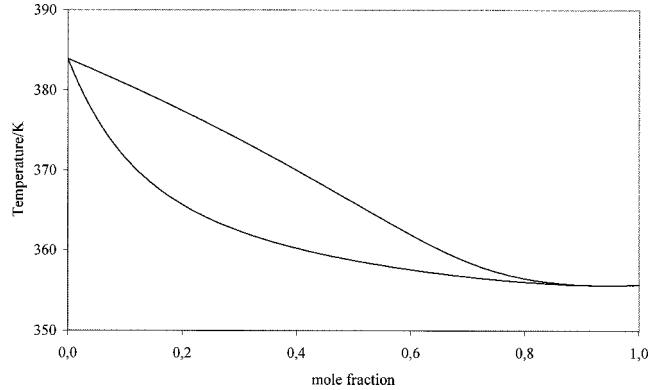
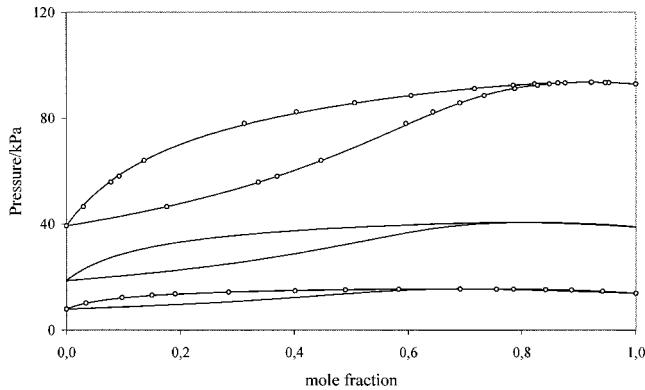


Table 3.27. 2-Methyl-2-propanol–ethylbenzene

Components			References		
2-Methyl-2-propanol, C <sub>4</sub> H <sub>10</sub> O [75-85-4]			<sup>1</sup> P. Oracz, Int. DATA Ser., Sel. Data Mixtures, Ser. A <b>17</b> , 247 (1989).		
Reference vapor–liquid equilibrium data					
<i>T</i> /K = 313.15, Ref. 1		<i>T</i> /K = 343.15, predicted		<i>T</i> /K = 373.15, predicted	
<i>P</i> /kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1,calc</sub>	<i>P</i> /kPa	<i>x</i> <sub>1</sub>	<i>y</i> <sub>1</sub>
2.873	0.00000	0.00000	11.33	0.00	0.00000
5.578	0.03806	0.4923	21.46	0.05	0.4927
6.866	0.06650	0.5909	28.07	0.10	0.6258
8.093	0.10970	0.6637	32.83	0.15	0.6906
8.838	0.14450	0.6975	36.49	0.20	0.7304
9.639	0.20640	0.7359	39.44	0.25	0.7583
9.987	0.24350	0.7521	41.89	0.30	0.7796
10.257	0.27900	0.7649	43.99	0.35	0.7968
11.107	0.39660	0.7969	45.82	0.40	0.8115
11.611	0.48170	0.8151	47.46	0.45	0.8245
12.100	0.58390	0.8354	48.95	0.50	0.8365
12.582	0.68240	0.8566	50.33	0.55	0.8479
12.848	0.74570	0.8726	51.62	0.60	0.8591
13.080	0.79780	0.8883	52.87	0.65	0.8705
13.315	0.84960	0.9073	54.09	0.70	0.8825
13.488	0.89670	0.9288	55.29	0.75	0.8955
13.696	0.95650	0.9648	56.49	0.80	0.9100
13.787	1.00000	1.00000	57.68	0.85	0.9266
			58.87	0.90	0.9463
			60.03	0.95	0.9702
			61.12	1.00	1.0000

<i>Q</i> <sub>1</sub> =0.370	$\sigma_1=0.13 \text{ kPa}$	<i>Q</i> <sub>0</sub> =0.373	$\sigma_0=0.13 \text{ kPa}$	<i>Q</i> <sub>0</sub> =0.3112	<i>Q</i> <sub>0</sub> =0.244	<i>Q</i> <sub>0</sub> =0.268
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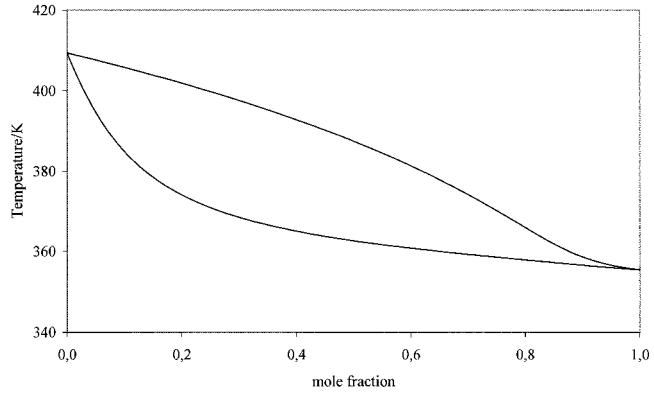
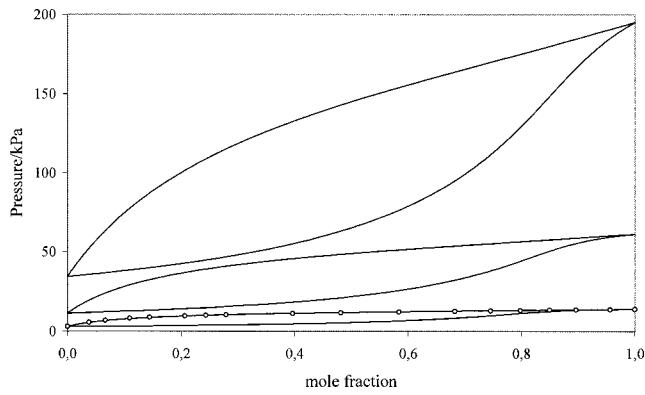


Table 3.28. 3-Pentanol–benzene

Components			References					
3-Pentanol, C <sub>5</sub> H <sub>12</sub> O [584-02-1]	Benzene, C <sub>6</sub> H <sub>6</sub> [71-43-2]		<sup>1</sup> J. M. Rhodes, T. A. Griffin, M. J. Lazzaroni, V. R. Bhethanabotla, and S. W. Campbell, Fluid Phase Equilib. <b>179</b> , 217 (2001).					
Reference vapor–liquid equilibrium data								
T/K = 313.15, Ref. 1			T/K = 333.15, predicted			T/K = 353.15, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>
24.309	0.0000	0.0000	73.26	0.00	0.0000	179.61	0.00	0.0000
24.083	0.0298	0.0168	72.20	0.05	0.0298	176.82	0.05	0.0320
23.777	0.0621	0.0278	70.92	0.10	0.0497	173.61	0.10	0.0577
23.499	0.1006	0.0369	69.54	0.15	0.0654	170.11	0.15	0.0802
23.016	0.1506	0.0459	68.07	0.20	0.0791	166.35	0.20	0.1011
22.537	0.2009	0.0534	66.50	0.25	0.0920	162.32	0.25	0.1214
22.036	0.2519	0.0603	64.81	0.30	0.1046	158.03	0.30	0.1418
21.506	0.2918	0.0655	62.99	0.35	0.1175	153.45	0.35	0.1628
20.859	0.3510	0.0733	61.01	0.40	0.1310	148.55	0.40	0.1849
20.246	0.4009	0.0802	58.86	0.45	0.1456	143.32	0.45	0.2086
19.617	0.4509	0.0878	56.51	0.50	0.1618	137.74	0.50	0.2345
19.579	0.4509	0.0878	53.93	0.55	0.1801	131.78	0.55	0.2631
18.872	0.5008	0.0963	51.10	0.60	0.2013	125.41	0.60	0.2954
18.029	0.5514	0.1062	47.98	0.65	0.2265	118.62	0.65	0.3325
17.104	0.6015	0.1179	44.56	0.70	0.2572	111.37	0.70	0.3756
16.061	0.6517	0.1322	40.79	0.75	0.2959	103.64	0.75	0.4270
14.864	0.7018	0.1504	36.63	0.80	0.3466	95.41	0.80	0.4896
13.519	0.7523	0.1746	32.06	0.85	0.4162	86.64	0.85	0.5678
11.940	0.8026	0.2084	27.03	0.90	0.5184	77.30	0.90	0.6688
10.159	0.8520	0.2581	21.49	0.95	0.6839	67.38	0.95	0.8052
8.064	0.9020	0.3422	15.41	1.00	1.0000	56.84	1.00	1.0000
6.233	0.9399	0.4570						
4.691	0.9707	0.6316						
2.960	1.0000	1.0000						

$Q_1 = 0.275$	$\sigma_1 = 0.13 \text{ kPa}$
$Q_0 = 0.275$	$\sigma_0 = 0.13 \text{ kPa}$
	$Q_0 = 0.206$
	$Q_0 = 0.134$
	$Q_0 = 0.161$

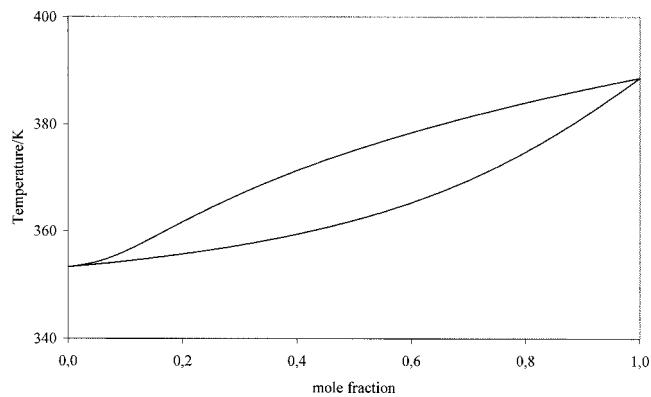
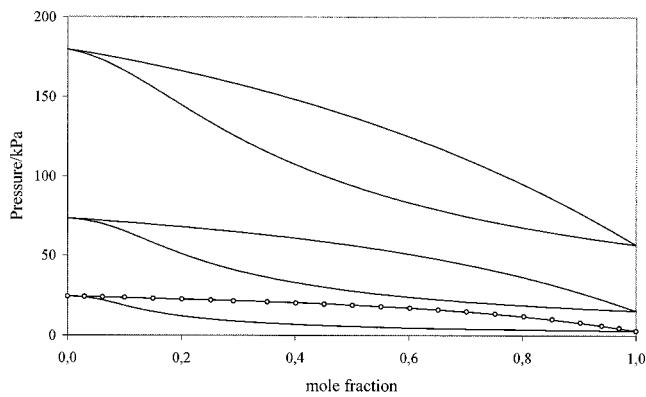


Table 3.29. 2-Methyl-2-butanol–benzene

Components			References					
2-Methyl-2-butanol, C <sub>5</sub> H <sub>12</sub> O [75-85-4] Benzene, C <sub>6</sub> H <sub>6</sub> [71-43-2]			<sup>1</sup> J. M. Rhodes, T. A. Griffin, M. J. Lazzaroni, V. R. Bhethanabotla, and S. W. Campbell, Fluid Phase Equilib. <b>179</b> , 217 (2001).					
Reference vapor–liquid equilibrium data								
T/K = 313.15, Ref. 1			T/K = 343.15, predicted			T/K = 373.15, predicted		
P/kPa	x <sub>1</sub>	y <sub>1,calc</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>	P/kPa	x <sub>1</sub>	y <sub>1</sub>
24.527	0.0000	0.0000	73.91	0.00	0.0000	181.22	0.00	0.0000
24.489	0.0304	0.0282	74.08	0.05	0.0468	181.16	0.05	0.0468
24.374	0.0614	0.0469	73.65	0.10	0.0794	180.21	0.10	0.0853
24.166	0.1006	0.0640	72.91	0.15	0.1054	178.67	0.15	0.1191
23.836	0.1513	0.0809	71.98	0.20	0.1280	176.68	0.20	0.1503
23.258	0.2300	0.1020	70.87	0.25	0.1489	174.30	0.25	0.1801
22.889	0.2759	0.1131	69.62	0.30	0.1691	171.58	0.30	0.2094
22.671	0.3005	0.1189	68.21	0.35	0.1892	168.53	0.35	0.2389
22.194	0.3505	0.1308	66.64	0.40	0.2098	165.15	0.40	0.2691
21.663	0.4005	0.1431	64.90	0.45	0.2316	161.43	0.45	0.3006
21.075	0.4504	0.1562	62.97	0.50	0.2551	157.38	0.50	0.3338
21.017	0.4509	0.1563	60.83	0.55	0.2809	152.96	0.55	0.3695
20.331	0.5011	0.1708	58.45	0.60	0.3100	148.17	0.60	0.4083
19.549	0.5526	0.1877	55.81	0.65	0.3433	142.98	0.65	0.4509
18.721	0.6011	0.2061	52.88	0.70	0.3824	137.37	0.70	0.4984
17.738	0.6517	0.2291	49.62	0.75	0.4293	131.32	0.75	0.5521
16.644	0.7011	0.2566	46.02	0.80	0.4872	124.80	0.80	0.6136
15.369	0.7519	0.2926	42.02	0.85	0.5609	117.79	0.85	0.6852
13.912	0.8003	0.3380	37.58	0.90	0.6586	110.26	0.90	0.7701
12.242	0.8525	0.4068	32.68	0.95	0.7951	102.17	0.95	0.8728
10.358	0.9016	0.5047	27.25	1.00	1.0000	93.50	1.00	1.0000
8.663	0.9407	0.6266						
7.201	0.9711	0.7738						
5.677	1.0000	1.0000						

$Q_1 = 0.261$	$\sigma_1 = 0.09 \text{ kPa}$
$Q_0 = 0.261$	$\sigma_0 = 0.08 \text{ kPa}$
	$Q_0 = 0.192$
	$Q_0 = 0.120$
	$Q_0 = 0.157$

